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Enclosed please find the required number of copies of the ONR Annual Technical Report and the ONR Annual Publication/Patents/Presentations/Honors Report as stipulated for the following ONR research contract.

TITLE: Theoretical Search for Supercapacitors
Semiconductors
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ONR O&T NO. 414-Q-013---02
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If there are any questions or comments on the material contained in these two documents, please contact me at (919) 515-5247.

I am very appreciative of the support provided for this research. Upon examination of the material contained in these reports, you will see that substantial progress has been made during the last annual funding period.

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A Theoretical Search for Supervelocity Semiconductors

M.A. Littlejohn and K.W. Kim, Principal Investigators

Department of Electrical and Computer Engineering

North Carolina State University

Raleigh, North Carolina 27695-7911

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a. **Papers Submitted to Refereed Journals (and not yet published)**

L.F. Register, M.A. Littlejohn and M.A. Strosio, "Path-Integral Monte Carlo Calculation of Real Self-Energies of Free and Confined Carriers," accepted for publication in Superlattices and Microstructures, 1991.

D.L. Woolard, H. Tian, R.J. Trew, M.A. Littlejohn and K.W. Kim, "A New Non-parabolic Hydrodynamic Model for Electron Transport in Semiconductors, accepted for publication in Phys. Rev. B.

H. Tian, K.W. Kim and M.A. Littlejohn, "An Investigation of Doping Profile Variations on AlGaAs/GaAs High Electron Mobility Transistor Performance," accepted for publication in J. Appl. Phys.

D.L. Woolard, R.J. Trew and M.A. Littlejohn, "Effect of Contact Regions on Transit Time and Velocity Overshoot in GaAs n^+-n-n^+ Structures, submitted to IEEE Trans. on Microwave Theory and Techniques.

D.L. Woolard, M.A. Littlejohn and R.J. Trew, "Impact of K-Space Transfer and Band Nonparabolicity on Velocity Overshoot in a GaAs Ballistic Diode," accepted for publication in Semicond. Sci. Technol.

K.W. Kim, M.A. Littlejohn, M.A. Strosio and G.J. Iafrate, "Transition from LO-Phonon to SO-Phonon Scattering in Mesoscale Structures," accepted for publication in Semicond. Sci. Technol.

H. Tian, K.W. Kim, and M.A. Littlejohn, "Ensemble Monte Carlo Study of A Novel Heterojunction Real-Space Transfer Logic Transistor (RSTLT)," accepted for publication in IEDM Technical Digest.

H. Tian, K.W. Kim, M.A. Littlejohn, S.M. Bedair and L. Witkowski, "Two-Dimensional Analysis of Short-Channel Delta-Doped GaAs MESFETs," submitted to IEEE Trans. on Electron Devices.

D.L. Woolard, M.A. Littlejohn and R.J. Trew, "The Role of Band Non-parabolicity in Negative Differential Conductivity of GaAs FETs," to be submitted to IEEE Trans. on Elec. Dev.

W.C. Koscielniak, M.A. Littlejohn and J.L. Pelouard, "Performance Limitations of Metal-Semiconductor-Metal Photodetectors," to be submitted to the Journal of Optical and Quantum Electronics.

W.C. Koscielniak, M.A. Littlejohn and J.L. Pelouard, "Simulation of an InGaAs/InAlAs MSM Photodetector," to be submitted to Electronics Letters.

b. Papers Published in Refereed Journals

K.W. Kim, M.A. Strosio, and J.C. Hall, "Frequencies of Confined Longitudinal-Optical Phonon Modes in Short-Period Strained Semiconductor Superlattices," *Proceedings of the SPIE International Symposium on Optical & Optoelectronic Applied Science and Engineering*, **1336**, 43 (1990).

M.A. Strosio, K.W. Kim, and J.C. Hall, "Variation in Frequencies of Confined Longitudinal-Optical Phonon Modes due to Changes in the Effective Force Constants Near Heterojunction Interfaces," *Superlattices and Microstructures*, **7**, 115 (1990).

M.A. Strosio, K.W. Kim, M.A. Littlejohn and H. Chuang, "Polarization Eigenvectors of Surface-Optical Phonon Modes in a Rectangular Quantum Wire," *Phys. Rev. B*, **42**, 1488 (1990).

H. Tian, K.W. Kim and M.A. Littlejohn, "Influence of DX-Centers and Surface States on Delta-Doped High-Electron-Mobility Transistor Performance," *J. Appl. Phys.*, **69**, 4123 (1991).

M.A. Strosio, K.W. Kim and M.A. Littlejohn, "Theory of Optical Phonon Interactions in a Rectangular Quantum Wire," *Proceedings of the International Society of Optical Engineering*, **1362**, 566 (1991).

K.W. Kim, H. Tian, and M.A. Littlejohn, "Analysis of Delta-Doped and Uniformly-Doped HEMTs by Ensemble Monte Carlo Simulation," *IEEE Trans. Electron Devices*, **ED-38**, 1737 (1991).

L.F. Register, M.A. Strosio and M.A. Littlejohn, "Constraints on the Polar-Optical-Phonon Influence Functional in Heterostructures," *Phys. Rev. B*, **44**, 3850 (1991).

M.A. Strosio, G.J. Iafrate, K.W. Kim, M.A. Littlejohn, H. Gronkin, and G. Maracus, "Transition from LO Phonon Scattering to SO Phonon Scattering in Polar Semiconductor Superlattices," *Appl. Phys. Lett.*, **59**, 1093 (1991).

c. Books (and sections thereof) Submitted for Publication

None

d. Books (and sections thereof) Published

M.A. Littlejohn, J.L. Pelouard, W.C. Koscielniak and D.L. Woolard, "Device Simulation Augmented by the Monte Carlo Method," Computational Electronics: Semiconductor Transport and Device Simulation, K. Hess, J.P. LeBurton and U. Ravaioli, eds., Kluwer Academic Publishers, pp. 69-75, 1991 - Book Chapter.

D.L. Woolard, M.A. Strosio, M.A. Littlejohn, R.J. Trew and H.L. Grubin, "A New Non-parabolic Hydrodynamic Transport Model with Quantum Corrections," Computational Electronics: Semiconductor Transport and Device Simulation, K. Hess, J.P. LeBurton and U. Ravaioli, eds., Kluwer Academic Publishers, pp. 59-62, 1991 - Book Chapter.

W.C. Koscielniak, M.A. Littlejohn and J.L. Pelouard, "Physical Speed Limits of Metal-Semiconductor-Metal Photodetectors," Gallium Arsenide and Related Compounds 1990, Institute of Physics Conference Series No. 112, K.E. Singer, editor, Institute of Physics, New York, 112, 613 (1990) - Book Chapter.

D.L. Woolard, H. Tian, M.A. Littlejohn, R.J. Trew and K.W. Kim, "The Application of Monte Carlo Techniques in Advanced Hydrodynamic Transport Models," Monte Carlo Device Simulation: Full Band and Beyond, K. Hess, ed., Kluwer Academic Publishers, Boston, MA, 1991.

e. Patents Filed

"A Heterojunction Real-Space Transfer Logic Transistor"

Patent disclosure in preparation

f. Patents Granted

None

g. Invited Presentations at Topical or Scientific/Technical Society Conferences

W.C. Koscielniak, M.A. Littlejohn and J.L. Pelouard, "Physical Speed Limits of Metal-Semiconductor-Metal Photodetectors," presented at the 17th International Symposium on Gallium Arsenide and Related Compounds, Jersey, Channel Islands, 24-27 September 1990.

M.A. Strosio, K.W. Kim and M.A. Littlejohn, "Theory of Optical-Phonon Interactions in a Rectangular Quantum Wire," presented at the SPIE International Conference on Physical Concepts of Materials for Novel Optoelectronic Device Applications II: Device Physics and Applications, Aachen, Federal Republic of Germany, October 1990.

h. Contributed Presentations at Topical or Scientific/Technical Society Conferences

K.W. Kim, M.A. Strosio and J.C. Hall, "Frequencies of Confined Longitudinal-Optical Phonon Modes in Short-Period Strained Semiconductor Superlattices," presented at the SPIE International Symposium on Optical and Optoelectronic Applied Science and Engineering, San Diego, CA, July 1990.

M.A. Strosio, G.J. Iafrate, K.W. Kim, M.A. Littlejohn, H. Gronkin and G. Maracus, "Transition from LO-Phonon Scattering to SO-Phonon Scattering in Polar Semiconductor Superlattices," presented at the Workshop on Compound Semiconductor Microwave Materials and Devices, Fort Lauderdale, FL, February 1991.

M.A. Stroschio, K.W. Kim and Amit Bhatt, "Electron-Optical-Phonon Scattering Rates in Rectangular Quantum Wire," presented at the Annual March Meeting of the American Physical Society, St. Louis, MO, March 1991.

D.L. Woolard, R.J. Trew and M.A. Littlejohn, "Effect of Contacts on Transit Time and Velocity Overshoot in GaAs n^+-n-n^+ Structures," presented at the Workshop on Compound Semiconductor Microwave Materials and Devices, Fort Lauderdale, FL, February 1991.

i. Honors/Awards/Prizes

None

j. Graduate Students and Postdoctorals Supported under the CRP for the year ending, 1 October, 1991.

D.L. Woolard - PhD student

W.C. Koscielniak - PhD Student (PhD degree awarded in June 1991)

H.Kim - PhD student

H. Tian - Visiting Research Assistant Professor

Annual Report To

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for

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Submitted by

North Carolina State University
Department of Electrical and Computer Engineering
Raleigh, North Carolina 27695-7911

For the Period January 1, 1991- December 31, 1991



Dr. M.A. Littlejohn
Principal Investigator
Soc. Sec. No. 242-60-6419
(919) 737-5247



Dr. K.W. Kim
Principal Investigator
Soc. Sec. No. 211-62-7519
(919) 737-5229

Submitted October 1991

EXECUTIVE SUMMARY

This document presents an annual report to the Office of Naval Research for a research program entitled "A Theoretical Search for Superspeed Semiconductors." This program has been funded by ONR since 1974 in the Department of Electrical and Computer Engineering at N.C. State University. The research has resulted in more than 75 refereed publications and numerous conference presentations from its inception. Major contributions to the field of hot electron transport and semiconductor device modeling have been achieved, new computational methods have been developed (e.g., path integral Monte Carlo techniques), and the work has helped stimulate commercial ventures in the applications of quaternary semiconductor materials to electronic and optical devices. In addition, there have been twenty-six Ph.D. and M.S. students who have received degrees at N.C. State University with research support from this contract. Three visiting faculty members from Japan came to the University to work with the faculty investigators supported under this ONR contract during the 1979-1983 time period. A visiting professor from the French CNRS Microstructures and Microelectronics Laboratory in Bagneux (near Paris) spent a sabbatical year at N.C. State during 1988-89, and he devoted full-time working on this program at no cost to ONR. During the current funding period, a visiting scholar from China is a member of our research group working on projects which directly impact this ONR program. Furthermore, we expect to add a new Visiting Research Assistant Professor this year to enhance our efforts in band structure calculations for quantum transport and mesoscopic devices.

The initial phases of this work centered around development of Monte Carlo simulation techniques which allow the study of detailed physics of hot electron transport in a variety of compound semiconductor materials. The original emphases were concerned with electronic materials phenomena. Later work considered the utilization of these materials in realistic device structures where physical boundary conditions must be imposed on the carrier transport. More recently, the work has focused on the domain of ultra small materials and device phenomena where microscopic non-local transient effects such as velocity overshoot, ballistic and nearly ballistic

transport, and quantum transport become important or dominant. During the past four years we have published new research results on applications of the Feynman "integral over paths" approach to quantum transport as well as the study of hot electron effects in new device structures, such as the hot electron spectrometer, heterojunction bipolar transistor, small dimension metal-semiconductor-metal photodetectors, and delta-doped high electron mobility transistors. Also, we have been exploring some new approaches to device modeling which combine the Monte-Carlo method with the method of moments of the Boltzmann transport equation (hydrodynamic transport model) for studying specific device structures, such as small-dimension n^+-n-n^+ majority carrier devices and the high electron mobility transistor. During the past year we have incorporated quantum correction terms into the hydrodynamic model and applied this model to resonant tunneling structures. Quite recently, we have applied a new ansatz distribution function as a constitutive relation to close the moment equations in the hydrodynamic transport model. Initial results of this approach have been physically satisfying and computationally promising. A comprehensive formulation of this new model will be published in the Physical Review in January, 1992. New work on the theory of optical phonon modes in heterostructures has demonstrated the importance of the effects of reduced dimensionality on transport dominated by the LO phonon interaction near heterointerfaces. As a result of this work, a new concept for velocity enhancement in pseudomorphic device structures is proposed for the new research program. Finally, we have developed a concept for a new device structure, which we call the real space transfer logic transistor (RSTLT). Preliminary results for this device predict a switching speed less than 3ps. These results will be presented at the International Electron Devices Meeting (IEDM) in December.

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Appendix A: List of Refereed Publications on This Program Since 1975.

Appendix B: Papers Published During Contract Period.

Appendix C: Resumes of Principal Investigators.

1.0 Introduction

In October 1974, the Office of Naval Research initiated sponsorship of a basic research program in the Department of Electrical and Computer Engineering (ECE) at North Carolina State University. The general goal of this research program has been and continues to be the investigation of high-speed carrier transport in III-V compound semiconductors, III-V alloy materials, other advanced electronic and optical materials, and novel device structures which utilize these materials. Four faculty members at N.C. State have been primarily involved in and supported by this project. They are M.A. Littlejohn, J.R. Hauser and T.H. Glisson, presently Professors in the ECE Department, and Dr. K.W. Kim who joined the ECE faculty in August 1988. Dr. Kim has served as a PI on the effort since January 1989 and is now a major contributor to these efforts. This research program has made significant contributions to the understanding and knowledge base of hot electron transport in materials and devices. It has provided scientific guidance to the U.S. Navy in the formulation of a part of its basic and applied research program. Numerical concepts developed under this project have been transferred to other Universities, including the University of Illinois, and we continue these interinstitutional collaborations. During the past year, faculty members and graduate students have spent time at the National Center for Computational Electronics at the University of Illinois (with Professor K. Hess). Also, collaborations with Dr. H.L. Grubin of Scientific Research Associates, Inc., Dr. M.A. Stroscio and Dr. G.J. Iafrate of the U.S. Army Research Office in the area of quantum transport in semiconductor devices have been strengthened. Dr. Iafrate, Dr. Stroscio, and Dr. Grubin are Adjunct Professors in the Electrical and Computer Engineering department at North Carolina State University. In addition to those directions, our research results have helped stimulate commercial ventures, particularly in the development of GaInAsP-based materials and devices. To-date, this program has resulted in 68 refereed publications in the literature, 6 additional manuscripts are currently in press, and 5 manuscripts have been submitted or are in preparation for submission to the technical literature. A listing of these publications is given in Appendix A. In addition, numerous invited talks and presentations have been given at conferences and workshops throughout the United States and in other countries. The program has contributed significantly to the educational program at N.C. State University with more than thirty Ph.D., M.S., and undergraduate students having received support under this ONR contract. Currently, three Ph.D. students are working toward their degrees on this project. Two of these Ph.D. students are U.S. Citizens. A visiting scholar from China is also working on research related to this program. We are now recruiting another Visiting Research Assistant Professor who can extend our capabilities into the areas of band structure effects and quantum transport in mesoscopic systems.

2.0 Research Results

2.1 Background

Since its inception, semiconductor technology has been stimulated by requirements for electronic systems with ever-increasing capabilities to process information faster, more functionally and more efficiently. These requirements have motivated the scaling-down of integrated circuit (IC) device dimensions into the submicron (less than ten thousand angstroms) and ultrasubmicron (less than one thousand angstroms) regions. Today, we have entered an era where nanostructure physics and fabrication motivate our research efforts in semiconductor electronics [1]. As fabrication technology has allowed such devices to be realized, many new and fundamental questions have emerged concerning the underlying physics of small (atomic level) dimensions in semiconductor devices. Important issues now under consideration for ultrasubmicron devices include nonequilibrium transport dealing with such topics as quasi-ballistic transport, overshoot phenomena and quantum transport. A great deal of progress has been achieved in our understanding of these important device effects, although major work remains to be done as our ability to fabricate very small electronic device structures continues to expand and mature [2,3].

The ability to fabricate small devices has been continually refined over the last fifteen years through impressive improvements in materials growth technologies. Molecular beam epitaxy (MBE), metalorganic chemical vapor deposition (OMCVD), and atomic layer epitaxy (ALE) have provided the ability to fabricate a wide variety of materials and heterostructure combinations with near perfect interfaces, doping control and compositional uniformity with atomic level dimensions. The development of ALE may very well prove to be the ultimate growth technology since it allows the deposition of one monolayer of device quality material through a controllable, self-limiting mechanism, and is especially useful for the deposition of heterojunctions [4]. The ability to grow layers with dimensions of a few angstroms opens the realm of quantum transport to experimental study and verification. Thus, topics resulting from size quantization in condensed matter must be investigated from theoretical viewpoints with tools which are either partially developed or through the development of new tools which are not now available. Quantization effects arising from geometrical size constraints, proximity effects resulting from closely packed arrays of devices, and general solid-state considerations not heretofore considered questionable (effective mass approximation, the role of interfaces and the like) must be addressed from a fundamental point of view. Moreover, from a device physics viewpoint, it is desirable to have a microscopic description of the physics of small dimensions which is amenable to phenomenological treatment, so that its properties can be meaningfully incorporated into futuristic device concepts and simulation.

Theoretical methods to address carrier transport have also progressed rapidly over the last ten-fifteen years, in a manner similar to research in semiconductor thin film epitaxial growth technology. In fact, this is a natural progression in many ways and is to be expected. The progress achieved in materials growth of structures with quantum dimensions dictates that new approaches be developed and refined to study quantum transport phenomena. However, a significant change in research direction is now warranted. Past transport theory and device modeling approaches have relied on particle or quasi-particle approaches where the electrons are treated as rigid mobile entities which undergo interactions with the transport medium. The treatment of the interaction often involves wave concepts. However, the model is basically a particle model. In the current regime of quantum transport, we may no longer be able to consider the carriers as particles. It is quite likely that their physical behavior will be governed either partially or completely by wave phenomena (i.e., electromagnetic and quantum mechanical effects).

The quasi-particle methods attempt to retain as much of the classical formalism as possible in order to be able to express results in terms of parameters which are of the greatest experimental interest, such as carrier velocity and diffusion constant. This is a flexible approach. However, much care is required to ensure that all important effects are properly included because of the approximations involved in the formulations. On the other hand, more fundamental quantum approaches, such as operator-eigenfunction methods, adhere closely to the actual quantum states present in the device structure when scattering is not included. Scattering processes (dissipation) can be added using perturbation theory from quantum mechanics. These techniques can obtain the greatest sensitivity to the resulting carrier confinement and the lattice potentials. However, they are relatively inflexible in studying non-linear dynamical properties in the presence of strong dissipation, such as is present in the electron-phonon interaction at high electric fields.

Another approach to quantum transport relies on the "integral over paths" method, originally proposed by Dirac and formulated by Feynman [5]. Path integral methods rely on an influence functional technique in which the source of the dissipation has been integrated over all phonon modes. This results in a model influence functional where the phonon-scattering dissipation can be represented as an interaction with a collection of harmonic oscillator modes in which the translational invariance of the carriers is preserved. The resulting model includes constant or oscillatory electric and magnetic fields, carrier screening, scattering and dissipation, carrier confinement, background temperature and initial conditions can be dealt with as readily as for a free particle [6].

The work at N.C. State University supported by the ONR under the current contract has progressed over the past sixteen years from the realm of particle models to quasi-particle models to quantum transport models. We have relied primarily on the Monte Carlo method to study and

solve transport problems in III-V compound semiconductors. Our techniques for modeling materials physics and device phenomena extend to device dimensions around one thousand angstroms [7-8], and we are confident in these models for predicting steady state and transient device effects down to these dimensions. However, in order to remain in the forefront of transport physics and device research, we must continue and increase our progress into the realm where physical effects can be studied in device regions with dimensions less than one thousand angstroms.

As one new direction for our research, we have chosen to pursue the path integral method. This is in contrast to other methods now being studied and supported by ONR, such as the application of the density matrix formalism and Wigner distribution function approaches including the use of moment equations [9]. We have made substantial progress in the path integral approach during the past five years and we believe that path integral methods can play an increasingly more significant role in developing an understanding of quantum transport in devices. Currently, we are aware of only one other U.S. university program directed toward applying the path integral method to semiconductor devices. This is the program at the University of Illinois under the direction of Prof. Karl Hess. Our program is very complimentary to the one at Illinois, and we are in fact collaborating with those personnel through the use of the NSF Supercomputing Center and the National Center for Computational Electronics there. One of our former students who finished his Ph.D. degree in 1990 has joined Prof. Hess' group and thus we expect this interaction to increase. We propose to spend a major effort collaborating with Prof. Hess' group in applying the path integral to specific device structures such as mesoscopic devices [10] during the next year, thereby further establishing its utility as a method for modeling quantum transport in devices. In addition, we will continue to explore the Monte Carlo transport method for study of novel device structures where theoretical underpinning is required. One particular class of devices which we will continue to study is based on hot electron injection across potential barriers where the transport mechanisms which determine device behavior are poorly or incompletely understood. Of great importance here is the fact that these devices offer the potential to compare experiment and theory. Also, these devices can be used to aid in our understanding of quasi-ballistic transport [3]. For example, we have explored the concept that ballistic-like behavior can be predicted even when scattering effects are significant [11]. The type of scattering and the range of carrier energies are critical in this regime. Another novel class of structures which will also be studied in detail by the Monte Carlo method is based on the rapidly-emerging pseudomorphic or strained-layer devices. These structures permit extended compositional ranges and, thus, have a number of potential advantages such as higher transconductance and channel carrier density. Recent studies on the strain-induced piezoelectric fields have opened yet another possibility in realizing ultra-fast switching devices, resulting in an increased importance on the study of carrier transport in these devices. Other novel

devices which will be analyzed include delta-doped field-effect transistors and quantum well structures, based on studies which have begun the past year. For example, we have proposed a new transistor structure - the real space transfer logic transistor (RSTLT) - which has a predicted switching speed of less than 3ps. If verified, this will be the fastest room temperature logic device yet reported. Finally, we will incorporate Monte Carlo methods into the quasi-particle approach based on moments of the Boltzmann transport equation with quantum mechanical corrections. Preliminary results show the utility of this approach for modeling microwave and millimeter wave devices which are important to the DoD's MMIC program.

We want to re-iterate the important interactions which have developed between our research group and other researchers during the last year. These interactions increase the impact of this program on the field of semiconductor device physics and allow our research efforts to be far more productive through increased intellectual efforts and enhanced facilities and resources. During the 1990-1991 funding periods, we have intensified our research collaborations with Prof. K. Hess at the University of Illinois, Dr. H. Grubin of Scientific Research Associates, and Drs. M. Strosio and G. Iafrate of the U.S. Army Research Office. These research collaborations have resulted in several joint publications based on mutual research interests, expertise and capabilities. There have been several visits between these laboratories and the logistics for increased collaborations are excellent. Also, we have very recently initiated an interaction with Dr. Doran Smith of ETDL, Fort Monmouth to verify the operation of the RSTLT.

2.2 Summary of Research Results

2.2.1 Path-Integral Monte Carlo (PIMC) Research for Ultra-Small Device Applications

This section will provide a summary of work concluded during the past year on the continued development of Path-Integral Monte Carlo (PIMC) methods for the study of the electronic properties of ultrasmall devices. The application of PIMC is based on the Feynman path-integral formalism of quantum mechanics. The following summary represents work done in collaboration with Dr. M.A. Strosio of the U.S. Army Research Office and Dr. L.F. Register of the University of Illinois. Dr. Register obtained his Ph.D. from N.C. State University and is now a Post-Doctoral Fellow at Illinois. The work deals with constraints on the polar-optical phonon influence functional in heterostructures which arise from conservation relationships for certain physical quantities in the PIMC formulation. The work is theoretical and formal; however, it has more practical applications since it provides a basis for estimation of the influence functional from limited knowledge of the spatial confinement of individual phonon branches. The results can help to expand our knowledge of electron-phonon interactions in heterostructures.

The *Feynman path-integral* (FPI) formulation of quantum mechanics allows formal inclusion of carrier phonon coupling to all orders in the coupling potential via the *influence functional* [12,13]. For this reason, the FPI has been extended to the study of confined carriers in ultrasmall heterostructure geometries [18], including recent advances in numerical methods [19-21]. However, in heterostructures, beyond the confinement of carriers, the confinement of phonons should be considered as well. Here, this latter confinement effect on the influence functionals for polar coupling of carriers to longitudinal-optical (LO) phonons is considered, without assuming any specific functional form for the phonon modes. In Section (a), the influence functional is defined in terms of the carrier-phonon modes. In Section (b), the influence functional is defined in terms of the carrier-phonon interaction Hamiltonian. In Section (c), it is shown that the partial contributions to the total influence functional from the individual branches of the LO-phonon spectrum are related and constrained by conservation relations. In Section (c), it is also shown that these conservation relations lead to the familiar results of Feynman [14,15] in the bulk crystal-limit, and that for heterostructures they provide a basis for estimation of the influence functional from limited knowledge of the spatial confinement of the individual phonon branches.

(a) Path-Integral Formalism

Consider a coupled carrier-phonon system with quantum mechanical Hamiltonian of the form

$$\mathcal{H} = \frac{\hbar^2}{2m} \nabla_r^2 + \mathcal{V}(r) + \sum_m \left(\frac{\hbar^2}{2} \frac{d^2}{d\xi_m^2} + \omega_m^2 \xi_m^2 + \phi_m(r) \xi_m \right) \quad (1)$$

where r is the carrier coordinate, ξ_m are the phonon coordinates, $\hbar\omega_m$ are the uncoupled phonon energies, and $\phi_m(r)$ are real functions characterizing the carrier position dependence of the carrier-phonon interaction. For this system, the equilibrium density matrix for the carrier averaged over the phonon coordinates and subject to a Maxwell-Boltzmann distribution in energies at temperature T is given by

$$\rho(r, r'; T) = \int_{r'}^r \exp \left\{ -\frac{\hbar/k_B T}{\hbar} \int_0^1 \left[\frac{1}{2m} |\dot{r}(t)|^2 + \mathcal{V}[r(t)] \right] dt \right\} \mathcal{F}[r(t)] \mathcal{D}r(t) \quad (2)$$

in the FPI formalism [13]. Here, " $\int_{r'}^r \mathcal{D}r(t)$ " signifies an integral over all paths from r' to r that are continuous functions of time, r' and $\mathcal{F}[r(t)]$ is the *influence functional*. $\mathcal{F}[r(t)]$ accounts for coupling between the carriers and phonons to all orders in the coupling potential and is given by [15]

$$\mathcal{F}[r(t)] = \exp \left\{ \sum_{m=1}^{\mathcal{M}} \frac{1}{4\hbar\omega_m} \int_0^{\hbar/k_B T} \int_0^{\hbar/k_B T} \phi_m[r(t)] \phi_m[r(t')] \left[\frac{e^{-\omega_m |t-t'|} + e^{\omega_m |t-t'| - \hbar/k_B T}}{1 - e^{\hbar\omega_m/k_B T}} \right] dt' dt \right\} \quad (3)$$

Equilibrium, rather than time-dependent, conditions are considered here for compatibility with existing numerical methods for performing carrier real self-energy calculations in confined geometries [19,21]. However, the calculations performed here can be adapted easily to the time-dependent case.

(b) Conservation Relations

For polar coupling of carriers to phonons, LO or otherwise, the interaction Hamiltonian for each phonon mode is

$$g_l^{(I)} = \frac{Z}{4\pi\epsilon} \sum_l \frac{(r-r_l)_j}{|r-r_l|^3} Z_l \sqrt{\frac{\hbar}{2M_l\omega_m}} \Phi_{m,l,j} (a_m^\dagger + a_m), \quad (4)$$

where ϵ is the free-space dielectric constant; z is the carrier charge; r_l , M_l and Z_l are the equilibrium position, mass and effective charge (the measure of ionization) of the l th ion, respectively; $\Phi_{m,l,j}$ are the normalized classical lattice vibrational modes of the crystal lattice as a discrete function of the mode, ion, and direction, respectively; the subscript j on a vector indicates the dot product of that vector with the unit vector in the j th direction; and a_m^\dagger and a_m are the raising and lowering operators, respectively [22]. Thus, in terms of the vibrational modes $\Phi_{m,l}$, the coupling functions $\phi_m(r)$ of Eqs. (3) and (5) are

$$\phi_m(r) = \frac{z}{4\pi\epsilon} \sum_{l,j} \frac{(r-r_l)_j}{|r-r_l|^3} \left(\frac{Z_l}{\sqrt{M_l}} \Phi_{m,l,j} \right), \quad (5)$$

where the relationship $\xi_m = \sqrt{\hbar/2\omega_m} (a_m^\dagger + a_m)$ has been used. Of course, knowledge of $\phi_m(r)$ is still limited by knowledge of $\Phi_{m,l,j}$, of which here only the following is claimed: for any crystal structure, the classical vibrational modes form a mathematically complete set of functions over the lattice degrees of freedom and, thus are subject to the orthogonality condition

$$\sum_m \Phi_{m,l,j} \Phi_{m,l',j'} = \delta_{l,l'} \delta_{j,j'} \quad (6)$$

where δ is the Kronecker delta function [23].

Having obtained the coupling functions $\phi_m(r)$ in terms of the classical vibrational modes $\Phi_{m,l,j}$, Eq. (5), the same now can be done for the influence functional $\mathcal{F}[r(t)]$ of Eq. (3). For any single branch of the LO-phonon spectrum ν of near uniform energy $\hbar\omega_\nu$, the spatial correlation of $\phi_{m,\nu}(r)$ encountered on the right-hand-side (RHS) of Eq. (3) becomes

$$\sum_{m_v} \phi_m(r) \phi_m(r') = \left(\frac{z}{4\pi\epsilon} \right)^2 \sum_{l, l' j j'} \frac{(r - r_l)_j (r' - r_{l'})_{j'}}{|r - r_l|^3 |r' - r_{l'}|^3} \left(\frac{Z_l Z_{l'}}{\sqrt{\mathcal{M}_l \mathcal{M}_{l'}}} \sum_{m_v} \Phi_{m, l j} \Phi_{m, l' j'} \right) \quad (7)$$

Though Eq. (6) is exact only for a sum over all modes, for an entire branch of the phonon spectrum, including perhaps noncoupling phonon modes that can therefore be included and weighted as desired, it is reasonable to expect the correlation function $\sum_{m_v} \Phi_{m, l j} \Phi_{m, l' j'}$ to remain short range in the displacement $r_l - r_{l'}$. Neglecting this displacement relative to $r - r'$ and accepting an uncertainty in ion position r_l of a single lattice primitive unit cell, transforms Eq. (7) to the form

$$\sum_{m_v} \phi_m(r) \phi_m(r') \approx \frac{z^2}{4\pi\epsilon^2 |r - r'|} \left[\frac{1}{\Gamma_v(r, r')} \right] \quad (8)$$

where

$$\frac{1}{\Gamma_v(r, r')} \equiv \frac{1}{4\pi} \sum_{j j'} \int \frac{(\mathcal{R} - \mathcal{R}_l)_j}{|\mathcal{R} - \mathcal{R}_l|^3} \left[\frac{1}{\gamma_{v j j'}(\mathcal{R}_l)} \right] \frac{(\mathcal{R}' - \mathcal{R}_l)_{j'}}{|\mathcal{R}' - \mathcal{R}_l|^3} d^3 \mathcal{R}_l; \quad (9)$$

$$\frac{1}{\gamma_{v j j'}(r, r')} \equiv \sigma_{ion}(r) < \frac{Z_l Z_{l'}}{\sqrt{\mathcal{M}_l \mathcal{M}_{l'}}} \sum_{m_v} \Phi_{m, l j} \Phi_{m, l' j'} >. \quad (10)$$

Here, $\mathcal{R} = r/|r - r'|$, $\mathcal{R}' = r'/|r - r'|$ and $\mathcal{R}_l = r_l/|r - r'|$; $\sigma_{ion}(r)$ is the local ion density; and "<>" indicates an average over ions l within a lattice primitive unit cell centered at r , and lattice configurations in the case of alloys. Substituting the approximation of Eq. (8) into Eq. (3), the influence functional takes the form

$$\mathcal{F}[r(t)] \approx \exp \left\{ \frac{z^2}{16\pi\epsilon^2 \hbar} \int_0^{\hbar/k_B T} \int_0^{\hbar/k_B T} \frac{1}{|r(t) - r(t')|} \sum_v \frac{1}{\Gamma_v(r, r')} \left[\frac{e^{i\omega_v |t - t'|} + e^{i\omega_v T(t - t' - \hbar/k_B T)}}{\omega_v (1 - e^{i\omega_v \hbar/k_B T})} \right] dt' dt \right\}, \quad (11)$$

where all effects of phonon localization are isolated in the form factors $\Gamma_v(r, r')$ [24].

As for $\phi_m(r)$ before, the result of Eq. (11) for the influence functional $\mathcal{F}[r(t)]$ is limited by the degree of knowledge of the lattice vibrational modes $\Phi_{m, l j}$. Fortunately, employing the orthogonality condition of Eq. (6) *exactly*, it is demonstrated readily that the functions $\gamma_{v j j'}(r)$ obey the conservation relation

$$\sum_v \frac{1}{\gamma_{v j j'}(r)} = \delta_{j j'} \frac{1}{\gamma(r)}, \quad (12)$$

where

$$\frac{1}{\gamma(r)} \equiv \sigma_{ion}(r) < \frac{Z_l^2}{\mathcal{M}_l} > \quad (13)$$

is a material dependent quantity only. For $\Gamma_V(r, r')$, via Eq. (9), this conservation relation translates to

$$\sum_V \frac{1}{\Gamma_V(r, r')} = \frac{1}{\Gamma(r, r')}, \quad (14)$$

where

$$\frac{1}{\Gamma(r, r')} \equiv \frac{1}{4\pi} \int \frac{1}{\gamma(\mathcal{R}_J)} \frac{(\mathcal{R} \cdot \mathcal{R}_J) \cdot (\mathcal{R}' \cdot \mathcal{R}_J)}{|\mathcal{R} \cdot \mathcal{R}_J|^3 |\mathcal{R}' \cdot \mathcal{R}_J|^3} d^3 \mathcal{R}_J. \quad (15)$$

Further, as defined in Eq. (13), $\gamma(r)$ is just a spatially varying version of the usual density function encountered in conventional bulk polar optical scattering rate calculations, that for a pure binary crystal can be obtained phenomenologically from $\gamma^{-1} = \omega^2 \epsilon (\epsilon_\infty^{-1} - \epsilon_0^{-1})$, where ϵ_∞ and ϵ_0 are the relative high and low frequency dielectric constants, respectively [25]. For an alloy, a compositionally weighted averaged of the pure material values should provide a reasonable approximation. Therefore, with these conservation relations, if not for the explicitly frequency dependent terms in Eq. (11), knowledge of the material dependent quantity $\gamma(r)$ alone would be sufficient to completely determine the total influence functional. As is, these conservation relations still provide a basis for estimation of the influence functional from limited knowledge of the spatial confinement of the individual phonon branches.

(c) Examples

For comparison with previous results, consider the limiting case of the influence functional of a pure binary bulk semiconductor. For this case there is only one LO-phonon branch and, thus, the influence functional is completely determined by only that phonon branch's optical phonon energy and the conserved quantity $\Gamma(r, r')$ [26]. For a homogeneous material, from Eq. (15), this latter quantity is given by simply $\Gamma(r, r') = \gamma(r) = \gamma$. Employing the phenomenologically obtained value for γ given above, gives from Eq. (11) exactly the influence functional obtained by Feynman for coupling to polar-optical phonons in bulk semiconductors (after switching to SI units and removing the normalizations) [14, 15]. This agreement results despite the use of dissimilar physical models. Here, discrete dipoles and a finite Brillouin zone are considered. In contrast, Feynman employs the Frölich model of the lattice polarization for carrier-polar-optical-phonon coupling, that of approximating the crystal lattice as a continuum of dipole charge characterized by the density function γ and the vibrational frequency ω [25], and, consistent with this continuum approximation, an infinite Brillouin zone.

As a second example, chosen to illustrate a range of phonon confinement possibilities, consider an AlGaAs-GaAs heterostructure of arbitrary geometry. The total dipole charge densities

within both materials are readily available as described above. Therefore, given the conservation relation of Eq. (12), only estimates of the relative contributions of the individual phonon branches as a function of position are required for evaluation of the influence functional via Eqs. (9) and (11) [27]. To this end, for large energy separations between the LO-phonon branch in the GaAs and the AlAs-like LO-phonon branch in the AlGaAs, the penetration depth of the AlAs-like phonon modes into the GaAs should be small and in a first approximation, can be neglected. For small energy differences between the LO-phonon branch in the GaAs and the GaAs-like LO-phonon branch in the AlGaAs, the branch in the AlGaAs [28] no distinction need be made between these two branches, and thus, the degree of phonon confinement between these branches becomes a moot point. Therefore, within the GaAs only the LO-phonon branch need be considered and, thus, the total dipole charge density γ_{GaAs} need not be subdivided. Further, while two phonon branches still must be considered within the AlGaAs, the relative contributions of each phonon branch $\gamma_{\text{AlAs-like}}$ and $\gamma_{\text{GaAs-like}}$ to the total dipole charge density γ_{AlGaAs} are the same as those required for conventional alloy scattering rate calculations [22,29-33]. If the energy separation between the optical phonon branches of the adjacent materials is considered to be in an intermediate range, that is when it is too large to be neglected but too small to prevent significant penetration of the phonon modes through the material interfaces on the spatial scale of interest, still only estimates of the relative contributions of each phonon branch near the interfaces to the totals γ_{GaAs} and γ_{AlGaAs} are required, not absolute nor mode by mode estimates. Possible bases for such estimates are, for example, calculations of confined phonon modes and penetration depths of evanescent phonon modes, e.g., Refs. 34-37.

(d) Conclusion

The Feynman influence functional for polar coupling of carriers to confined phonon modes in heterostructures has been considered. It was found that the partial contributions to the total influence functional from the individual branches of the optical phonon energy spectrum are related and constrained by conservation relations, Eqs. (12) - (15). The derivation of these conservation relations required no specific functional form for the phonon modes; rather it employed only the inherent orthogonality and mathematical completeness of the classical vibrational modes over the crystal lattice degrees of freedom. In the bulk crystal limit these conservation relations lead to the familiar results of Feynman for heterostructures and these conservation equations provide a basis for estimation of the influence functional from limited knowledge of the spatial confinement of the individual phonon branches. Further, though the FPI formalism is considered here, it should be possible to apply similar reasoning to more conventional scattering rate calculations in heterostructures, as was done for optical phonon scattering in alloys previously [22].

2.2.2 A New Non-Parabolic Hydrodynamic Transport Model in Semiconductors

During the past year, we have made a major step towards the development of a more realistic hydrodynamic transport model for semiconductors which includes nonparabolic band structure effects. This model contains a much improved physical description of device phenomena in nanostructures than does current drift-diffusion-based models while it is much less computer-intensive than Monte Carlo device simulation models. Our approach has been accepted for publication in the Physical Review (see Section 2.3). This section will describe the details of the new hydrodynamic model and compare the results with the Monte Carlo method.

The model is based upon a unique derivation of the moments of the Boltzmann transport equation for the collisionless case (collisions are introduced later). This derivation implements an efficient and compact mathematical formalism appropriate for electrons under the influence of high electric fields and nonstationary conditions. The theoretical investigation also introduces a novel distributional form, with nonparabolic properties, to precisely define the resulting nonparabolic transport parameters. The final set of model equations are exhibited in a fashion to clearly show the new factors as corrections to the more familiar hydrodynamic model applicable for the constant effective mass case. In addition, results of an extensive investigation of the assumed ansatz distribution and resulting nonparabolic model parameters using an elaborate Monte Carlo model are described. The Monte Carlo technique was used to generate comparison electron distributions and exact values for the nonparabolic transport parameters for stationary and nonstationary electronic structures. In all cases, excellent agreement was found between the Monte Carlo calculated parameters and the derived nonparabolic model terms. The Monte Carlo calculations also revealed that the ansatz distribution represented a significant improvement over the more familiar displaced Maxwellian. Therefore, this new model should prove very valuable for studying novel electronic device structures operating under high bias conditions.

(a) General Moment Equations

Consider the collisionless Boltzmann transport equation (BTE) in terms of the phase-space variables (\vec{r}, \vec{k}, t) . The developments presented here are independent of the specific scattering phenomena which will be addressed later. Hence, the BTE is

$$\frac{\partial f}{\partial t} + \vec{u} \cdot \nabla_{\vec{r}} f + \frac{\mathcal{F}}{\hbar} \cdot \nabla_{\vec{k}} f = 0 \quad (1)$$

where $f(\vec{r}, \vec{k}, t)$ is some arbitrary electron distribution function. Invoking the effective-mass theorem [38] (also called the quasi-free-particle approximation [39]) for electron motion defines the electron momentum as $p = \hbar \vec{k}$ and identifies the electron group velocity as

$$\frac{\partial \mathbf{r}}{\partial t} = \mathbf{u}(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E}(\mathbf{k}). \quad (2)$$

The driving force on the electron is $\mathbf{F} = \partial \mathbf{p} / \partial t$ and the final form of Eq. (1) is established.

The overall goal is to study moments of the BTE, Eq. (1), for the case of nonparabolic conduction bands. Thus, the first step is to develop a general moment equation. This is achieved by multiplying Eq. (1) by an arbitrary vector (or scalar) operator $\Phi(\mathbf{k})$ and integrating with respect to \mathbf{k} to obtain

$$\int \Phi \frac{\partial f}{\partial t} d^3k + \int \Phi \mathbf{u} \cdot \nabla_{\mathbf{r}} f d^3k + \int \Phi \frac{\mathbf{F}}{\hbar} \cdot \nabla_{\mathbf{k}} f d^3k = 0. \quad (3)$$

By noting that Φ is a function of \mathbf{k} alone and invoking the assumption that f approaches zero rapidly enough in the limits of integration such that $\int \nabla_{\mathbf{k}} (\Phi f) d^3k$ is negligible [40], one obtains the general moment equation

$$\frac{\partial}{\partial t} \int \Phi f d^3k = -\nabla_{\mathbf{r}} \cdot \int \Phi \mathbf{u} f d^3k + \frac{\mathbf{F}}{\hbar} \cdot \int \nabla_{\mathbf{k}} \Phi f d^3k \quad (4)$$

in terms of the driving force \mathbf{F} , \mathbf{k} -space dependent electron velocity $\mathbf{u}(\mathbf{k})$ and an arbitrary vector moment operator $\Phi(\mathbf{k})$. Equation (4) represents the mathematical form required to develop the nonparabolic conservation or hydrodynamic transport equations.

For this nonparabolic model, the Kane energy band dispersion relation [38] for nonparabolic bands will be utilized. This relation is given by

$$\frac{\hbar^2 k^2}{2m^*} = \mathcal{E}(\mathbf{k}) (1 + \alpha \mathcal{E}(\mathbf{k})). \quad (5)$$

The specific choice of operators will determine what average physical quantity is conserved in each moment equation. For this work we have chosen the following operators for use in the generalized moment equation, eqn. (4) above.

$$\Phi_0(\mathbf{k}) = 1 \quad (6)$$

$$\Phi_1(\mathbf{k}) = \mathbf{u}(\mathbf{k}) = \frac{\hbar \mathbf{k}}{m^*} \quad (7)$$

$$\Phi_2(\mathbf{k}) = \mathcal{E}_c(\mathbf{k}) = \frac{m(\mathbf{k})}{Z} \mathbf{u}(\mathbf{k}) \cdot \mathbf{u}(\mathbf{k}) \quad (8)$$

where

$$m(\mathbf{k}) = m^* \sqrt{1 + \frac{2\alpha \hbar^2 k^2}{m^*}} \quad (9)$$

and

$$E_s(k) = E(k) \left(\frac{1 + \alpha E(k)}{1 + 2\alpha E(k)} \right) \quad (10)$$

These moment operators are not the standard ones traditionally used in the development of the hydrodynamic model. Their uniqueness and significance are discussed in detail in ref. 41.

By applying (6), (7), and (8) in (4), the nonparabolic hydrodynamic collisionless transport equations for conservation of particles, average momentum and average energy in Lagrangian form are:

$$\frac{\partial n}{\partial t} = -\nabla_r \cdot (nv) \quad (11)$$

$$\frac{\partial v}{\partial t} = -v \cdot \nabla_r v + \frac{\mathcal{F}}{m} = \frac{1}{nm} \cdot \nabla_r \cdot [\mathcal{P}_v], \quad (12)$$

$$\frac{\partial w}{\partial t} = -v \cdot \nabla_r w + \mathcal{F} \cdot v = \frac{1}{n} \nabla_r \cdot (v \cdot [\mathcal{P}_w] + q) \quad (13)$$

where;

$$n = \int f d^3k \quad (14)$$

$$nv = \int u(k) f d^3k \quad (15)$$

$$nw = \int \frac{m(k)}{2} u(k) \cdot u(k) f d^3k \quad (16)$$

$$\frac{n}{m} = \int \frac{f}{m(k)} d^3k \quad (17)$$

$$[\mathcal{P}_v] = m \int (u(k) - v)(u(k) - v) f d^3k \quad (18)$$

$$[\mathcal{P}_w] = \int m(k)(u(k) - v)(u(k) - v) f d^3k \quad (19)$$

$$q = \int \frac{m(k)}{2} (u(k) - v)(u(k) - v) \cdot (u(k) - v) f d^3k \quad (20)$$

Before this system of equations can be applied to the study of electron transport additional assumptions must be invoked to express Eqs. (17) - (20) in terms n , v and w . This mathematical

closure entails the use of specific fundamental physical properties to evaluate these parameters. Efforts have been made to express these parameters in a mathematical form which is as compact as possible. It is clear that the integral definitions consist primarily of terms involving $u(k)$ and differ from the definitions for the parabolic case only by the introduction of the nonparabolic mass $m(k)$ and the specific definition of the particle velocity $u(k)$. This property will be utilized in the next section to develop approximate expressions so that this nonparabolic form of the hydrodynamic equations may be used to study electron dynamics in realistic electronic structures.

(b) Nonparabolic Transport Model

The previous equations represent a general nonparabolic hydrodynamic transport model for electron transport in a single valley of GaAs. Additional assumptions or relationships are necessary to close the system of equations before they can be used to describe transport phenomenon. Specifically, one must either ignore one or more higher order terms in the formulation [42], have some previous knowledge for the equations of state [43,44], or assume some form of the electron distribution function in momentum space [45]. These are all acceptable methods of simplification and can lead to the same unique system of equations.

The use of a predefined distributional form is often viewed as being more restrictive and less general than some of the previous alternatives. Yet, many derivations, which seek to develop models applicable for more generalized distributions, partially implement closure relations with properties proven true only for specific distributional forms. Extending the electron transport model in this manner has merit and leads to results which are more physically accurate. However, mixing assumptions in this manner can obscure regions of validity for the complete model. Defining a specific form of the distribution function is the most complete approach and easiest to evaluate from both a physical and mathematical point of view. Therefore, this is the approach considered here.

The distribution most frequently chosen to describe nonequilibrium transport phenomenon is the displaced Maxwellian function. For the case of parabolic conduction bands this distribution function, in momentum space, is [45]

$$f_{dm}(k) = \frac{nf^3}{\left(2\pi m^* k_B T_e\right)^{3/2}} \exp\left[\frac{-k^2 |k - k_d|^2}{2m^* k_B T_e}\right], \quad (21)$$

where k_B is the Boltzmann constant, T_e is the temperature of the electron gas representing the spread of the distribution, and k_d is the displacement from $k = 0$ of the Maxwellian distribution. The previous distribution ignores any affect that Fermi-Dirac statistics may have on the total number of available electrons. Since this work is directed toward transport in conduction bands and it is a simple task to modify the normalization coefficient to include these Fermi effects, they

will be ignored throughout. This Maxwellian approach has been applied often in the analysis of such problems; however, for the case of nonparabolic bands Monte Carlo calculations indicate that such a distribution leads to a less than adequate treatment of the transport parameters of the hydrodynamic model.

In this derivation a unique treatment is proposed for closing the general moment equations for electron transport in GaAs. To articulate the basis of this approach, consider a form of the displaced Maxwellian distribution $\mathcal{F}_{dm}(u)$ transformed into velocity space such that $\mathcal{F}_{dm}(u)d^3u = f_{dm}(k)d^3k$ or specifically, $\mathcal{F}_{dm}(u) = |J_{dm}|f(u^{-1}(k))$. Here, the inverse function $u^{-1}(k)$ represents the function $u^{-1}(k) = k = g(u)$ where $g(u)$ is the correct mapping from momentum space to velocity space. Also, J_{dm} is the appropriate Jacobian transformation [46] from momentum space to velocity space. Defining this velocity space distribution in such a manner allows parametric definitions of the form $I = \int i(k)f_{dm}(k)d^3k$, similar to Eqs. (17) through (20), to be expressed in velocity space as $I = \int i(u^{-1}(k))\mathcal{F}_{dm}(u)d^3u$. Therefore, for the case of parabolic bands where the relationship between velocity space and momentum space is linear, $u(k) = (\hbar k)/m'$ and $|J_{dm}| = (m'/\hbar)^3$, this corresponding displaced Maxwellian distribution in velocity space is

$$\mathcal{F}_{dm}(u) = n \left[\frac{m}{2\pi k_B T_e} \right]^{3/2} \exp \left[\frac{-m' |u - v|^2}{2k_B T_e} \right] \quad (22)$$

where v now represents the average as well as the displacement under consideration in velocity space. Both Eq. (21) and Eq. (22) are symmetric about their displacements within their respective spaces and the average velocity v is equal to $(\hbar k_d)/m'$; therefore, Eq. (22) does represent a completely consistent transformation of Eq. (21) for the case of parabolic bands.

One would expect that, under the conditions of nonparabolic bands where the effective mass of the electron depends on its precise location in the conduction band, the use of constant m' would be insufficient. Also, another dilemma exists in defining a single temperature of the electron gas since it has been shown that two distinctly different temperatures tensors T_v and T_w occur for the case of nonparabolic bands. Thus, stationary Monte Carlo calculations and physical intuition suggests the following ansatz distribution.

$$\mathcal{F}_{nonpar}(u) = n \left[\frac{m_w(v, T_w)}{2\pi k_B T_w} \right]^{3/2} \exp \left[\frac{-m_w(v, T_w) |u - v|^2}{2k_B T_w} \right] \quad (23)$$

as a constitutive relation to close the moment equations for the case of nonparabolic energy bands. Here a single effective temperature T_w is still utilized. However, T_w , with a distinct w subscript,

has been chosen to replace T_e because $(3/2)k_B T_w$ (here T_w is defined from diagonal elements of the energy pressure $\langle P_w \rangle$) approximates the effective thermal energy well for the stationary transport case at moderate values of average energy. In addition, $m_w(v, T_w)$ has been introduced because, based on physical considerations, we expect a nonconstant average effective mass which should depend strongly on the spread or thermal component T_w of the true electron distribution and on the displacement in velocity space v .

In applying Eq. (23) to the integral definitions (14) - (20), it is correct to use $\mathcal{F}_{nonpar}(u)d^3u = f_{nonpar}(k)d^3k$, since \mathcal{F}_{nonpar} was postulated in velocity space from a distribution which contained this transformation property. However, the issue of transforming between momentum and velocity space for the case of nonparabolic bands involves very complicated nonlinear transformations. Thus, it is instructive to consider this issue briefly. Assume for the moment that a correct form for the distribution in momentum space is known and denote this distribution as $f_{nonpar}(k)$. To preserve the property $\mathcal{F}_{nonpar}(u)d^3u = f_{nonpar}(k)d^3k$ so that transforming integral definitions consists just of inverting the $i(k)$ in $I = \int f_{nonpar}(k) d^3k$, a new nonlinear transformation factor, J_{nonpar} , such that

$$\mathcal{F}_{nonpar}(u) = J_{nonpar} f_{nonpar}(u^{-1}(k)) \quad (24)$$

is needed. In Eq. (52), $u^{-1}(k) = k = g(u)$ is assumed to exist and to be a single-valued function of u . This can be shown to be true for transformations from a finite region about $k = 0$ in momentum space to a finite region about $u = 0$ in velocity space [47].

For the case of nonparabolic bands, defined by relation (5) and a resulting nonlinear momentum space velocity $u(k)$ given by Eq. (9), the appropriate factor is $J_{nonpar} = j_{nonpar}^{-1}$ where [46]

$$j_{nonpar} = \begin{vmatrix} \frac{\partial v_x}{\partial k_x} & \frac{\partial v_x}{\partial k_y} & \frac{\partial v_x}{\partial k_z} \\ \frac{\partial v_y}{\partial k_x} & \frac{\partial v_y}{\partial k_y} & \frac{\partial v_y}{\partial k_z} \\ \frac{\partial v_z}{\partial k_x} & \frac{\partial v_z}{\partial k_y} & \frac{\partial v_z}{\partial k_z} \end{vmatrix} \quad (25)$$

Using the definition of $u(k)$ given by Eq. (7) in Eq. (25) results in

$$j_{nonpar} = \left(\frac{\hbar}{m(k)} \right)^3 \begin{vmatrix} 1 + C(k)k_x^2 & C(k)k_x k_y & C(k)k_x k_z \\ C(k)k_y k_x & 1 + C(k)k_y^2 & C(k)k_y k_z \\ C(k)k_z k_x & C(k)k_z k_y & 1 + C(k)k_z^2 \end{vmatrix} \quad (26)$$

where

$$C(k) = - \frac{2\alpha \hbar^2}{m^* (1 + \frac{2\alpha \hbar^2 k^2}{m^*})} \quad (27)$$

The transform defined by Eq (26) is extremely complex. Also, it is obvious that completing the remaining determinate operation and performing the necessary functional substitution will introduce cross-coupled real space transformation factors. Therefore, to gain more insight in this investigation, the near equilibrium case will be considered where most of the electrons are near the conduction band minimum. For this case the off-diagonal terms may be neglected and Eq. (26) can be approximated to lowest order in k to obtain

$$j_{nonpar} = \left(\frac{\hbar}{m(u^{-1}(k))} \right)^3. \quad (28)$$

In order to proceed further, more information about the distribution in momentum space appropriate for nonparabolic bands is necessary. The concept of a Maxwellian function [48], where the distribution assumed is of the form $(n/I_n) \exp[-E(k)/(k_B T_e)]$ (where I_n is the appropriate normalization factor), will now be applied to generate a test distribution in momentum space to gain additional insight. Doing this and using the approximate definition for electron energy from Eq. (8) results in a simplified illustrative distribution, under displacement k_d of

$$f_{nonpar}(k) = \frac{n}{I_n} \exp \left[\frac{-m(k - k_d) u^2(k - k_d)}{2k_B T_e} \right]. \quad (29)$$

Using Eq. (57) as a test function, the transformation Eq. (52) yields

$$\mathcal{F}_{nonpar}(u) = \frac{n}{I_n} \left(\frac{m(u^{-1}(k))}{\hbar} \right)^3 \exp \left[\frac{-m(u_v^{-1}(k - k_d)) u_v^2(u_v^{-1}(k - k_d))}{2k_B T_e} \right] \quad (30)$$

where for this distribution $u^{-1}(k)$ represents the function $u^{-1}(k) = k = g(u)$ and $u_v^{-1}(k)$ represents some undefined function of the form $u_v^{-1}(k) = k - k_d = g(u \cdot v)$.

Examination of Eq. (30) reveals that the exponential argument is modulated by a function, $m(u_v^{-1}(k - k_d))$, which resembles an effective mass term with velocity displacement dependence.

The simplified \mathcal{F}_{nonpar} derived here does not exhibit the exact form of the ansatz distribution function defined by Eq. (23). However, the previous analysis does lend theoretical support to the idea of using the intuitively derived \mathcal{F}_{nonpar} of Eq. (23) as a tool to investigate nonequilibrium electron transport for the case of nonparabolic conduction bands. Indeed, later it will be shown that this distribution leads to excellent results for nonequilibrium transport in nonparabolic conduction bands.

Applying these relations and through much mathematical manipulation, the new collisionless nonparabolic hydrodynamic transport model equations are:

$$\frac{\partial n}{\partial t} = -\nabla \cdot (nv) \quad (31)$$

$$\frac{\partial v}{\partial t} = -v \cdot \nabla_r v + \frac{\mathcal{F}}{m^* \mu} - \frac{2}{3nm^*} \nabla_r \cdot \left[nV \left(w - \frac{m^*}{2} |v|^2 \right) \right] \quad (32)$$

$$\frac{\partial w}{\partial t} = -v \cdot \nabla_r w + \mathcal{F} \cdot v - \frac{2}{3n} \nabla_r \cdot \left[nV(w + \phi) \left(w - \frac{m^*}{2} |v|^2 \right) \right] \quad (33)$$

$$\mu(v, w) = 1 + 2\alpha \varepsilon(v, w) \left(w - \frac{m^*}{2} |v|^2 \right) + \frac{10\alpha^2}{3} \varepsilon(v, w)^2 \left(w - \frac{m^*}{2} |v|^2 \right)^2 + \alpha m^* |v|^2 \quad (34)$$

$$v(v, w) = \frac{\varepsilon(v, w)}{\mu(v, w)} \quad (35)$$

$$w(v, w) = \varepsilon(v, w) \left[1 + \frac{4\alpha}{3} \varepsilon(v, w) \left(w - \frac{m^*}{2} |v|^2 \right) + \alpha m^* |v|^2 \right] \quad (36)$$

$$\phi(v, w) = \frac{10\alpha}{3} (v(v, w))^2 \left(w - \frac{m^*}{2} v \cdot v \right) \left[1 + 14\alpha v(v, w) \left(w - \frac{m^*}{2} v \cdot v \right) \right] \quad (37)$$

where

$$\varepsilon(v, w) = \frac{1 - \frac{4\alpha}{3} w}{1 + \alpha m^* |v|^2} \quad (38)$$

The details of the derivation are presented in Ref. 41.

The nonparabolic model equations above have been written in a form so that for the parabolic case, $\alpha = 0$, it is easy to observe that $\mu = v = w = 1$ and $\phi = 0$. Then the parabolic model conveniently reduces to the more familiar classical hydrodynamic equations in Lagrangian form, as given by eqns. (11) — (20).

(c) Scattering and Transport Model Parameter Evaluation

The nonparabolic hydrodynamic model derived in the last section ignored any specific form of scattering mechanisms. This was done primarily to simplify the analysis and to allow for a clear focus on the transport parameters which evolve from the collisionless BTE for nonparabolic bands. To evaluate the results of the previous section one could assume a form for the scattering mechanism and then solve the resulting system of equations with appropriate boundary conditions (The authors have performed such a study [50]). Results for electron current could then be used to judge the macroscopic feasibility of the new nonparabolic model. However, the issue of choosing accurate forms for scattering terms is a complicated one and the specific form has a large influence on the results obtained. Therefore, a different initial approach will be followed. The specific approach will be to calculate the resultant nonparabolic parameters m^{**} , $[P_v]$, $[P_w]$ and q of the hydrodynamic model for various structures using an elaborate Monte Carlo model. Since the results of the previous section presented formulas for each of the model parameters in terms of average velocity v and average energy w , the values predicted by these formulas can easily be

compared to those from more elaborate and detailed Monte Carlo model. Taking this approach will give an excellent gauge of the accuracy of the terms of the model without the possible errors introduced by using incorrect forms for the loss mechanisms.

The first test applied was to generate the electron distribution and nonparabolic parameters, directly from their integral definitions (17) - (20), for a time steady-state constant field structure over a variety of electric field values using Monte Carlo techniques. For these stationary investigations, two independent Monte Carlo models were used to analyze electron transport in GaAs. Both of these models utilize single particle Monte Carlo procedures to improve computational accuracy and efficiency. The models incorporate three valley analytical band structures and included all the significant scattering mechanisms with polar optical intervally scattering. In addition, both models used the same material and physical parameters [51].

Under these stationary conditions, as can be observed directly from Eqs. (11) - (13) or indirectly in Eqs. (31) - (33), only the value of m'' will affect the final solution for transport. This is true because all the other terms are space differential in nature. However, as will be shown, these terms do have finite values which vary widely over the cases considered. Also, for these conditions, all the displacement terms (terms of form $\alpha m' |v|^2$ are found to be negligible). Hence, this is an excellent test for the accuracy of the derived nonparabolic model parameters and their dependence on energy temperature T_w . The test also reveals how well T_w is determined by its dependence on total kinetic energy, w , and the displacement kinetic energy term, $(m'/2) |v|^2$. An investigation into the true electron distribution is also very important since F_{nonpar} is instrumental in determining the final formulas for the nonparabolic terms.

The results of these stationary investigations, with the two independent Monte Carlo models in agreement, are presented in Figs. 1 - 4. Fig. 1 exhibits the resulting Monte Carlo generated distribution, the ansatz distribution \mathcal{F}_{nonpar} and the displaced Maxwellian distribution \mathcal{F}_{dm} along the direction of applied field, in velocity space, for two values of electric field. Here, the Monte Carlo distributions were obtained by sampling electrons which resided in a slice of velocity volume from the three dimensional velocity space. In the calculations, a limiting velocity v_s is used to define the size of the slice in the directions other than that of the electric field. v_s was chosen small enough to clearly and accurately show the velocity distribution and large enough for a practical simulation time.

Fig. 3 clearly indicates that the corrected electron distribution \mathcal{F}_{nonpar} is a distinct improvement over displaced Maxwellian. Using \mathcal{F}_{dm} results in a general tendency, for any select average velocity and energy, to overspread and place too many electrons in the tail of the distribution. Conversely, the improved distribution \mathcal{F}_{nonpar} retains more electrons closer to equilibrium. This result seems correct for the situation of an energy dependent effective particle mass (or nonparabolic conduction band) and is verified by the Monte Carlo generated distributed.

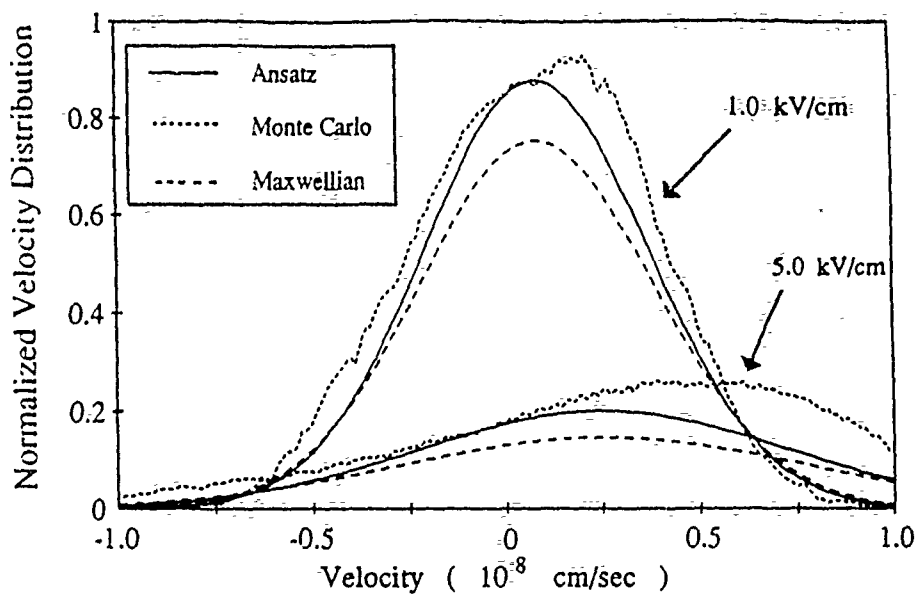


Figure 1: Normalized Γ valley velocity distribution functions resulting from the constant electric field values of 1.0 kV/cm and 5.0 kV/cm. The profiles are exhibited along the direction of net average velocity (along direction of applied field). All distributions shown are consistently normalized to contain an identical number of electrons.

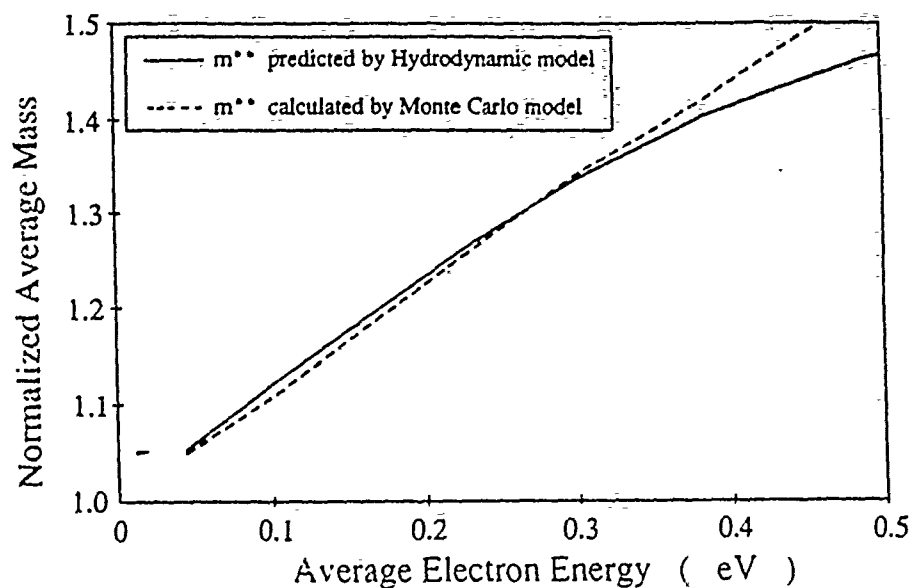


Figure 2: Average r valley effective mass, m^{**} , normalized by near equilibrium mass value of $m^* = 0.57 \times 10^{-31} \text{ kg}$ and plotted versus average electron energy, ω . These results were calculated for stationary transport conditions.

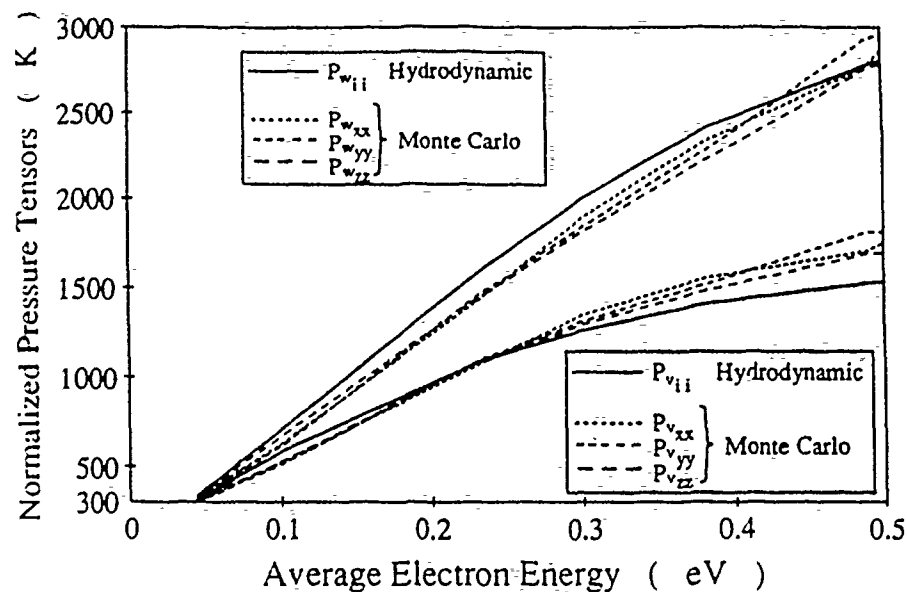


Figure 3: Velocity and energy Γ valley pressure tensors, normalized by nk_B , versus average electron energy. The off-diagonal terms are omitted because they are negligible (an order of magnitude smaller) compared to diagonal terms. These results were calculated for stationary transport conditions.

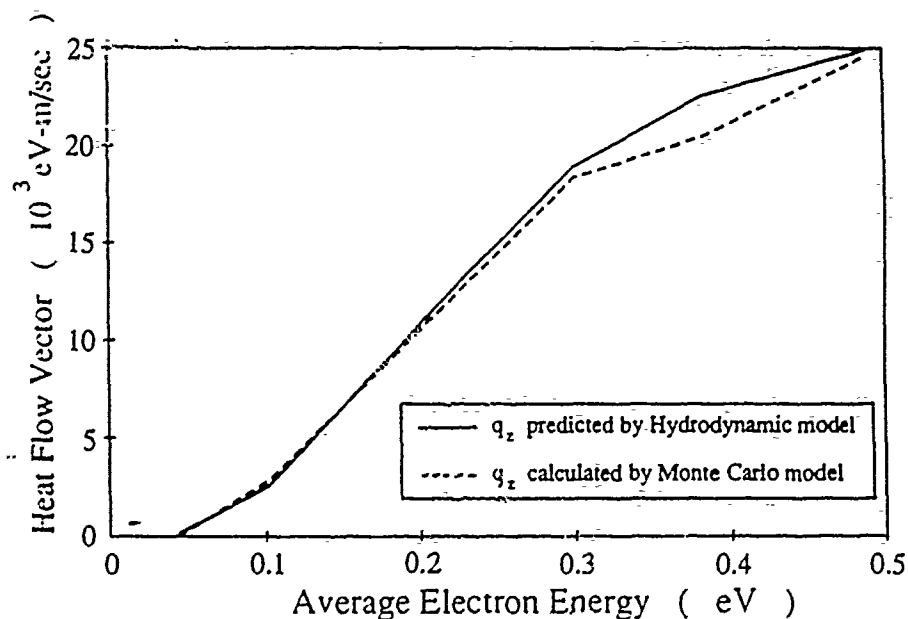


Figure 4: Γ valley heat flow vector along the direction of applied electric field, normalized by n , versus average electron energy. The other vector components are omitted because they are negligible compared to field direction component. These results were calculated for stationary transport conditions.

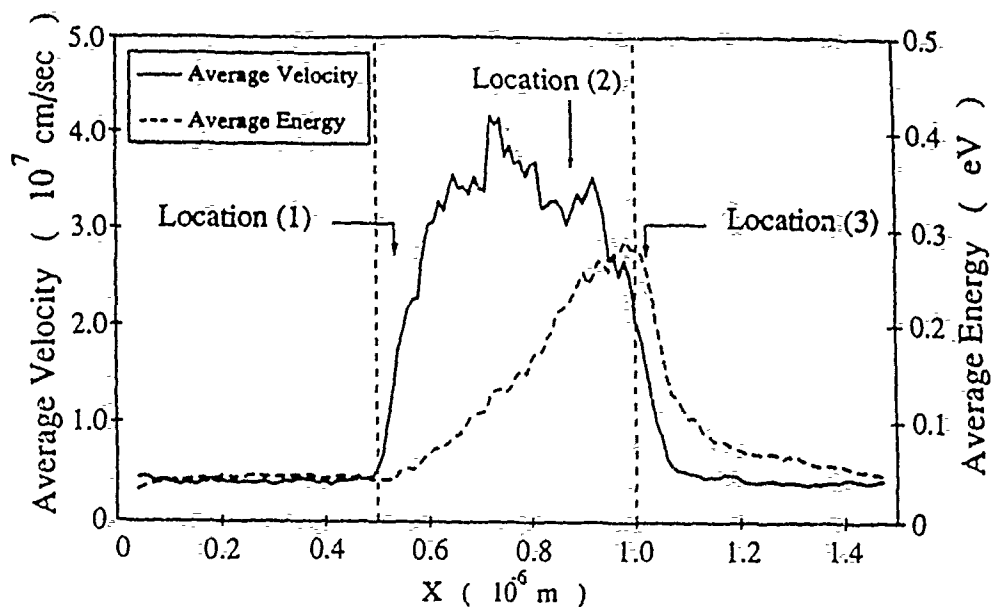


Figure 5: Γ valley average velocity and energy profiles through a submicron GaAs $N^+ - N^- - N^+$ ballistic diode-structure biased at 0.8 volts. The structure consists of $0.5 \mu\text{m}$ long source and collector regions doped 10^{17} cm^{-3} with a $0.5 \mu\text{m}$ active region doped 10^{13} cm^{-3} . The diagram also indicates three locations ($z = 0.53 \mu\text{m}$, $0.85 \mu\text{m}$ and $1.03 \mu\text{m}$) where the nonparabolic model transport parameters were investigated using the Monte Carlo method.

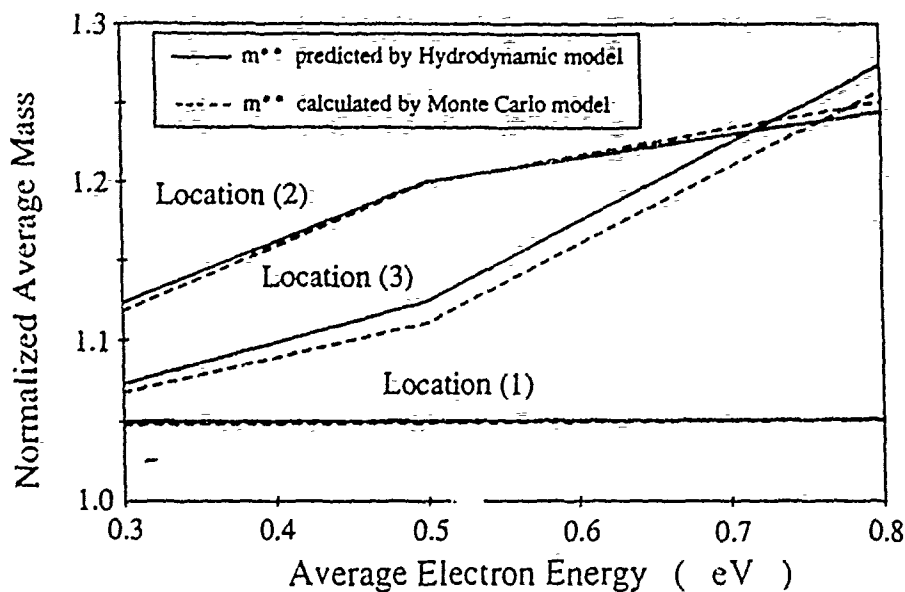


Figure 6: Normalized average Γ valley effective mass, at three locations within the ballistic diode, plotted as a function of applied bias.

The stationary results for a variety of electric field values, corresponding to the nonparabolic transport parameters, are presented in Figs. 2 - 4 and are plotted versus the average electron energy for each case. In each instance, the nonparabolic transport parameters predicted by the hydrodynamic model were calculated using the Monte Carlo values for average velocity v and average energy w since they are fundamentally dependent on these variables.

In general, the predictions supplied by the nonparabolic parameter are in excellent agreement with the results calculated by the Monte Carlo model. Fig. 2 shows that the values for the average effective mass m^{**} predicted by hydrodynamic model are essentially equal (less than 1 percent difference) to those calculated by the Monte Carlo model up to 0.4eV. Fig. 5, which gives both the momentum pressure $[P_v]$ and the energy pressure $[P_w]$, clearly shows that these tensors are approximated well by a diagonal matrix. Further, the diagonal elements for both are in very good agreement with the predictions made by the hydrodynamic model. Finally, Fig. 4 shows the comparison between the hydrodynamic model's values for the heat flow vector q and those calculated by Monte Carlo. These results also agree very well, which leads to a very important point. The nonzero expression for the heat flow vector was derived here from first principles for the nonparabolic conduction band case. It also represents the first nonequilibrium analysis for such a transport factor which is usually based on thermodynamics arguments. However, it should also be noted that for highly nonstationary conditions this term may need to be determined by higher moments of the BTE before it is accurate for transport simulations [52].

While the previous stationary results are very positive, they alone are not sufficient to insure the applicability of this new model to arbitrary electron device structures. Realistic device structures, operating under moderately high biases, always contain regions where transport occurs under nonstationary conditions. Hence, additional calculations were performed to determine the accuracy of the nonparabolic model subject to these conditions. The $n^+ - n - n^+$ ballistic diode, a simple prototypical submicron structure which has been extensively studied [53], was chosen as a test device.

A self-consistent ensemble Monte Carlo model was used to calculate the nonparabolic parameters for several strategically selected locations within this device as illustrated in Fig. 5. Specifically, locations were selected which would exhibit different types of nonstationary transport. At location (1) the electron gas is relatively cool with a low average energy, but, the average velocity is slightly ballistic. Converse to this, at location (3) the average energy remains high and the average velocity is low. Finally, location (2) represents a case where both gas parameters are elevated and are experiencing significant gradients.

The results of these nonstationary studies are presented in Figs. 6-9 where the various transport parameters are plotted as a function of applied bias. Summarizing the results, the transport parameters predicted by the hydrodynamic model are in very good agreement with the

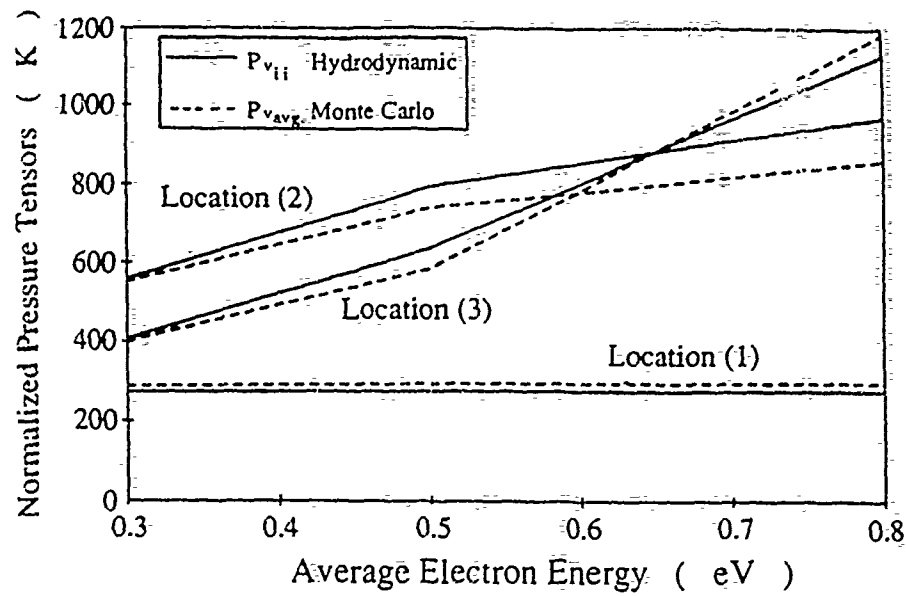


Figure 7: Normalized Γ valley velocity pressure, at three locations within the ballistic diode, plotted as a function of applied bias. $P_{v_{avg}}$ represents the average of the three diagonal components which were found from Monte Carlo calculations to be approximately equal. Off-diagonal terms were negligibly small.

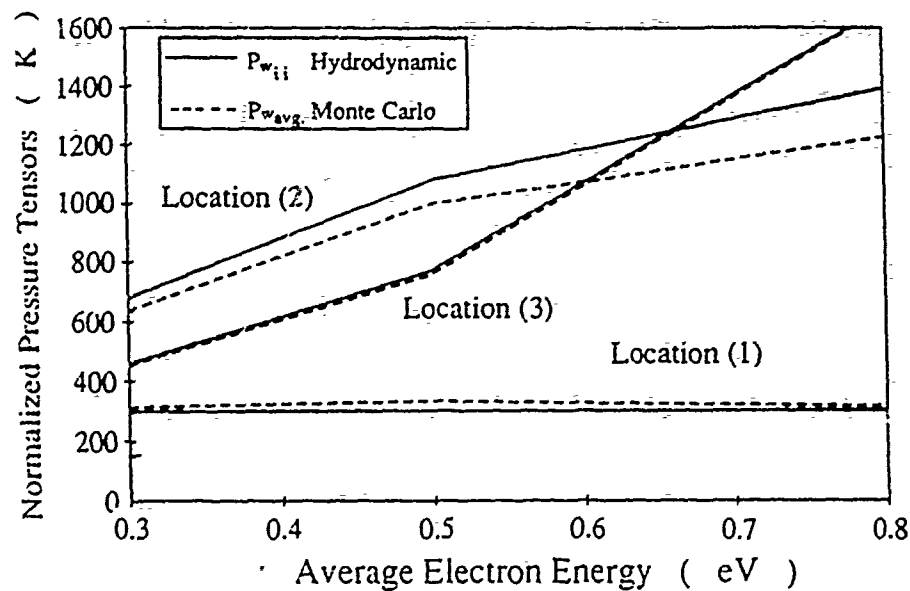


Figure 8: Normalized r valley energy pressure, at three locations within the ballistic diode, plotted as a function of applied bias. $P_{w_{avg}}$ represents the average of the three diagonal components which were found from Monte Carlo calculations to be approximately equal. Off-diagonal terms were negligibly small.

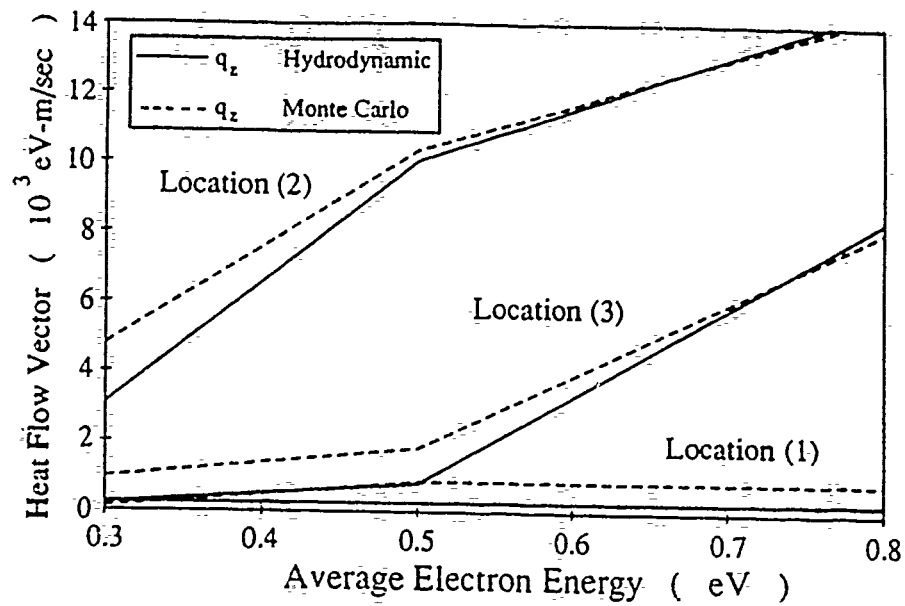


Figure 9: Γ valley heat flow vector along the direction of applied electric field, at three locations within the ballistic diode, plotted as a function of applied bias. The other components were found to be negligibly small.

direct Monte Carlo calculations. In fact, the agreement for all parameters are within 10 percent for the majority of the biases studied. In addition, the difference only rises slightly higher to approximately 20 percent (for the heat flow vector) at low biases where the accuracy of the Monte Carlo statistics are in question. The results agreed both qualitatively and quantitatively for all three locations and at all biases. Hence, all the results indicate this new nonparabolic hydrodynamic model can accurately approximate electron transport in realistic semiconductor devices.

(d) Conclusion

This section has presented a unique derivation for a new nonparabolic hydrodynamic transport model. This new approach utilized novel moment operators to reveal simplifying assumptions and to arrive at more compact mathematical formulation. This formulation was then used to postulate an improved ansatz distribution to close the moment equations and result in a model and nonparabolic transport parameters which accurately reflects transport of electrons in realistic semiconductor conduction bands. When combined with appropriate dissipation terms. This simplified model offers a computationally efficient method to model electron conduction in semiconductors. This type of model, which sacrifices some physical detail, leads to a more manageable mathematical problem with the potential of rapid solution generation using numerical methods.

Additionally, this section presents an extensive Monte Carlo based investigation into the applicability of this new model. The model parameters were tested in both stationary and nonstationary environments. In both cases the results are excellent. Hence, this model should prove instrumental in investigating novel electronic device structures. The model offers a method to better approximate electron transport with the potential of faster simulation times as compared to the more computationally intensive Monte Carlo technique.

2.2.3 Transport in Photoexcited Semiconductors

During the past four years, we have studied the transport of photoexcited carriers in semiconductors. We have explored the use of Monte Carlo simulation as well as quantum mechanical wave approaches to examine scattering effects and ballistic transport. The specific device which we have chosen to explore is the GaAs metal-semiconductor-metal (MSM) photodetector with a planar (low electrode capacitance) structure which is of interest for discrete applications and optoelectronic integrated circuits (OEICs).

Recently, based on the results of our Monte Carlo simulations (see refs. 46,47,54 and 56 in Appendix A), Prof. Mourou's research group at the University of Michigan have achieved a world-record GaAs detector performance. Using a MSM photodetector with 0.2 μm finger

spacing, a power bandwidth of 325 GHz was obtained. In last year's report, we predicted that such high bandwidths were achievable if parasitic effects could be minimized. The key to Prof. Mourou's results was the use of low-temperature MBE-grown GaAs to minimize the effects of parasitic circuit elements and hole transport delay times.

There are obvious benefits in fabricating MSM photodetectors on GaAs. The high electron velocity of GaAs (10^7 cm/sec) allows one to obtain high responsivity, and the relatively high hole velocity (3×10^6 cm/sec) makes this device extremely attractive for high-speed applications. Advances in GaAs device fabrication techniques and process compatibility of the MSM photodetector with existing IC processing are responsible for many applications of this device in its discrete or monolithic versions. However, the GaAs photodetector can only operate at wavelengths below about $0.87 \mu\text{m}$. The range of wavelengths acceptable by this detector is unfortunately incompatible with low loss transmission minima or current state-of-the-art optical fibers. The low loss minima of optical fibers at $1.3 \mu\text{m}$ and $1.55 \mu\text{m}$ can be used to advantage if we investigate semiconductors such as InGaAs. This semiconductor has even higher electron velocities than GaAs. However, holes in InGaAs move much more slowly than GaAs [54]. This implies that the InGaAs detector will be slower than GaAs although it operates at longer wavelengths. Although some tradeoffs will have to be made, there are interesting areas of applications for the InGaAs MSM photodetector. This year, we have begun simulations of InGaAs photodetectors for use at longer wavelengths. The following section summarizes the initial simulations of the InGaAs detector in an attempt to define its performance and limitations.

In Fig. 1 we show a schematic cross-section of an InGaAs MSM photodetector which we have investigated. Compositions of three epitaxial layers are chosen such that there is a perfect lattice match between these layers and the InP substrate. Thus, carrier trapping by defects created by lattice mismatch can be minimized. Since we already know that collection of slow holes generated deep beneath the surface in InGaAs can ultimately determine the speed of this device, the thickness of the active InGaAs layer is chosen to be $1 \mu\text{m}$. There is a minor responsivity loss associated with limiting the carrier generation depth to about $1 \mu\text{m}$. The doping densities of the active layer and the two remaining layers are dictated by current progress in film growth techniques. The donor doping densities of $5 \times 10^{14} \text{cm}^{-3}$ for InGaAs and $5 \times 10^{15} \text{cm}^{-3}$ for InAlAs are very close to current background densities of pure epitaxial layers grown by MOCVD. There is no straightforward way to determine how thick the InAlAs barrier enhancing layer should be. A semiconductor with a larger bandgap must be introduced between the InGaAs and the Schottky contact to lower the dark current. The thicker this barrier, the smaller will be the probability for carrier tunneling through the barrier. Hence, the dark current will be smaller. However it is also true that a thicker barrier would tend to keep photogenerated carriers inside the InGaAs for longer periods of time. Based on available experimental designs of InGaAs MSM photodetectors [55] we

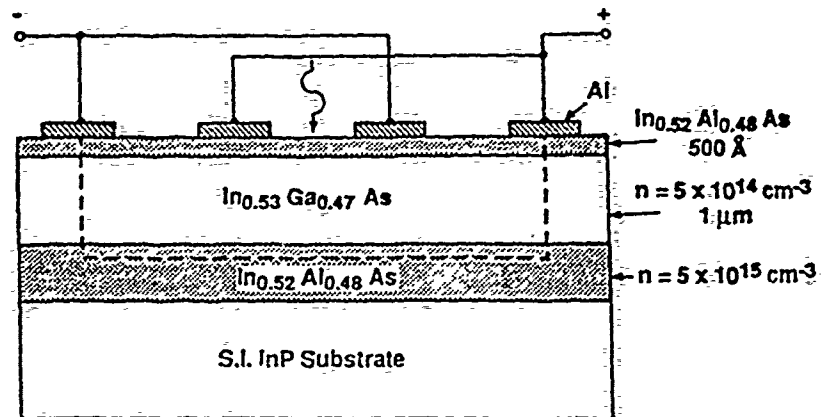


Figure 1: Cross-sectional view of InGaAs MSM photodetector. The top and bottom InAlAs layers are used to confine carrier generation to 1 μm thick InGaAs. The broken line represents the simulated area of the device.

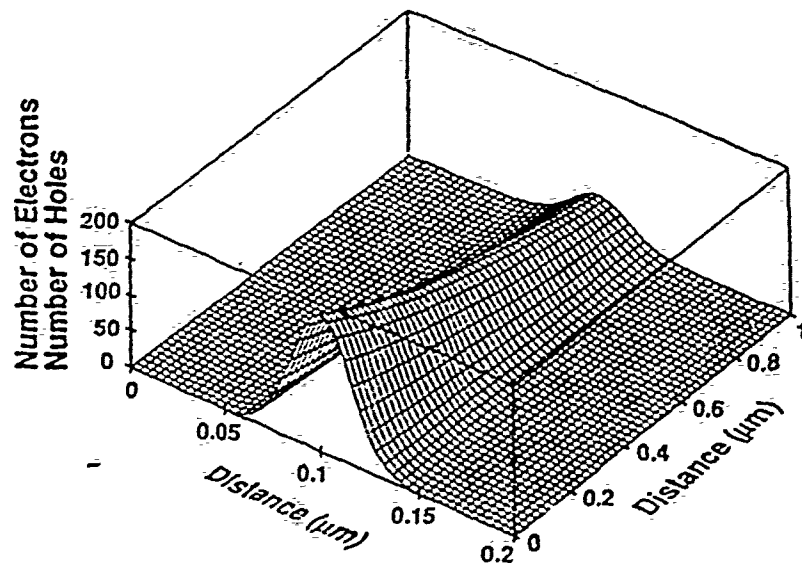


Figure 2 Two-dimensional initial pattern of generated electrons and holes. There are 2000 generated electron-hole pairs.

chose 500 Å for the thickness of the InAlAs barrier enhancing layer. A separate study will be necessary to determine the optimal barrier thickness. A sub-half micron distance between fingers is chosen since there are no known simulation results for such devices. All present photodetectors are usually fabricated with 1-3 μm distance between fingers. The simulation technique employed in the present studies does not permit the simulation of long devices due to a prohibitively long computation time. Therefore, the presented results are for a 0.2 μm detector.

The initial electron-hole pair distribution in InGaAs is determined by the finger spacing and wavelength of light. Since the spacing between fingers is smaller than the wavelength of light, there will be a diffraction pattern formed in the interfinger area. We approximate this pattern with a Gaussian exponentially decaying with depth as shown in Fig. 2. The exact pattern could be obtained from Maxwell's equations. The absorption coefficient for InGaAs used in generating the initial carrier pattern is $1.25 \times 10^4 \text{ cm}^{-1}$ [56]. The number of electron-hole pairs used in the simulation is 2000. We have performed simulations with various initial energies of electrons and holes or, alternatively various wavelengths of incident light.

The intrinsic time response shown in Fig. 3 is obtained from simulations with a wavelength of 1.55 μm . Thus, the electrons are generated with an initial energy slightly larger than the InGaAs bandgap. This curve displays similar features as the time responses for GaAs detectors, except for the change in time scale. Since the initial results revealed that it is necessary to increase the bias voltage to increase the detector speed, this simulation was performed for a bias voltage of 1.4 V. The InAlAs layer has been removed for these simulations. We see that this device is considerably slower than the GaAs device. As we have done for the GaAs photodetectors, discrete and monolithic versions of the detector are introduced. By comparing the time responses of these two versions of the photodetector, we notice only minor differences between them. This behavior is caused by a much slower intrinsic pulse for InGaAs than for GaAs. We deal with a parasitic circuit suitable for high frequencies, or suitable for generating short pulses, excited by a relatively slow current source. As a consequence, we cannot take advantage of monolithic integration of this device since reduction in values of the parasitics does not have much influence on the response. We see from Fig. 3 that it takes much longer than 25 ps for the output voltage to settle. The long tail associated with holes causes the bandwidth of the detector to decrease.

In Fig. 4 we show the output power spectra of an InGaAs MSM photodetector. One common feature of all curves is that for frequencies up to about 100 GHz there is little difference in output power of intrinsic, discrete, and monolithic detectors. Consequently the 3 dB bandwidth of 21.8 GHz for the intrinsic detector remains almost unchanged for the discrete and monolithic versions. We can make the following summary based on these initial results for the InGaAs MSM photodetector. The device is useful for detection of optical pulses at 1.55 μm . It is necessary to optimize the thickness of the barrier enhancing layer (InAlAs) in order to lower the dark current

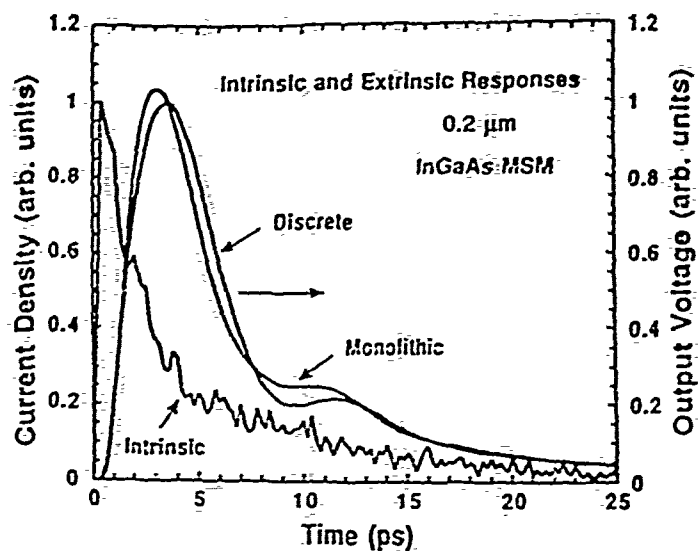


Figure 3 Simulated intrinsic and extrinsic response for an InGaAs photodetector. Much slower holes in InGaAs than in GaAs cause this device to have a long hole tail. This also results in very similar responses for the discrete and monolithic versions of the device.

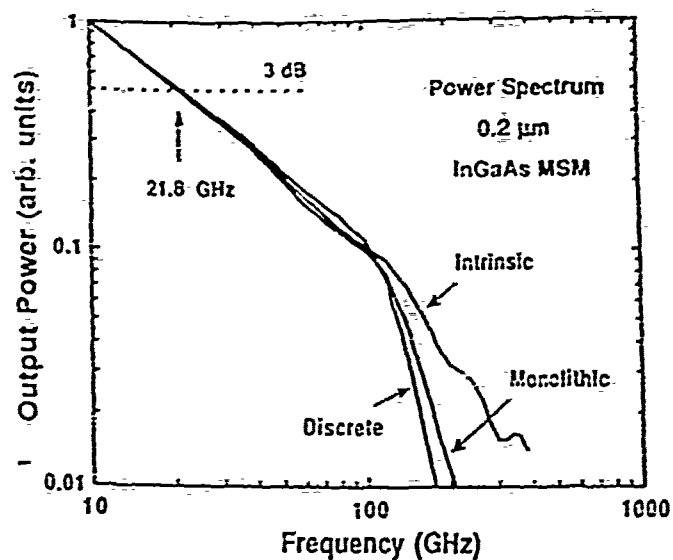


Figure 4 Power spectra of InGaAs MSM photodetector. The 3 dB frequency is 21.8 GHz for all considered versions.

without significant deterioration of electron collection. Although the small distance between fingers suggests possible use of small bias voltage, there is a speed deterioration associated with small bias. In order to remove slow holes and increase the device speed we must increase the bias voltage, which unfortunately, increases the dark current. The interdigitated pattern shows similar responses for the discrete and monolithic detectors.

2.2.4 Study of Delta-doped FET Structures

(a) Monte Carlo Simulation of Delta-Doped HEMT Structures

As a promising candidate for ultra-high speed and microwave applications, delta-doped FET structures are attracting considerable attention. By applying the delta-doping technique, devices (such as MESFETs, AlGaAs/GaAs based HEMTs, pseudomorphic HEMTs, and HBTs) can achieve improved performances. These include enhanced threshold voltage control, reduced trapping effects, better breakdown characteristics, and (most importantly) increased conducting channel electron density and more efficient utilization of introduced dopants. The resulting experimental devices show higher current drive capability, higher transconductance and higher frequency performance. In spite of continuing experimental interests in delta-doped structures, theoretical studies on these devices are rare and mainly first order (either analytical model or by drift-diffusion approximation). Theoretical study of electron transport properties in such structures is necessary in order to understand the mechanism of device operation, to further improve (optimize) device performance, and to exploit potential new device structures. During the past year, we have performed a systematic study of the delta-doped HEMT structures. In particular, the following issues are theoretically investigated for submicron AlGaAs/GaAs delta-doped HEMTs by ensemble Monte Carlo simulation:

- Comparative study of delta-doped and uniformly doped HEMTs — First, we compared the performances of experimentally available (from literature) submicron HEMTs and a comparable uniformly-doped HEMT and investigated mechanisms for the enhanced performance of delta-doped HEMTs. To correctly simulate the operations of practical devices, our Monte Carlo model includes the real-space transfer effect, the carrier degeneracy effect, and influences of DX centers and surface states in addition to all the scattering mechanisms (such as polar optical, intervalley, ionized impurity, electron-electron scatterings). A two-dimensional, self consistent Poisson equation solver is implemented in the program for accurately updating the electric field in the device. Our results reveal that the improvement in electron confinement in conducting channel (as shown in Fig. 1) and reduced peak channel electric field are the main reasons that produce

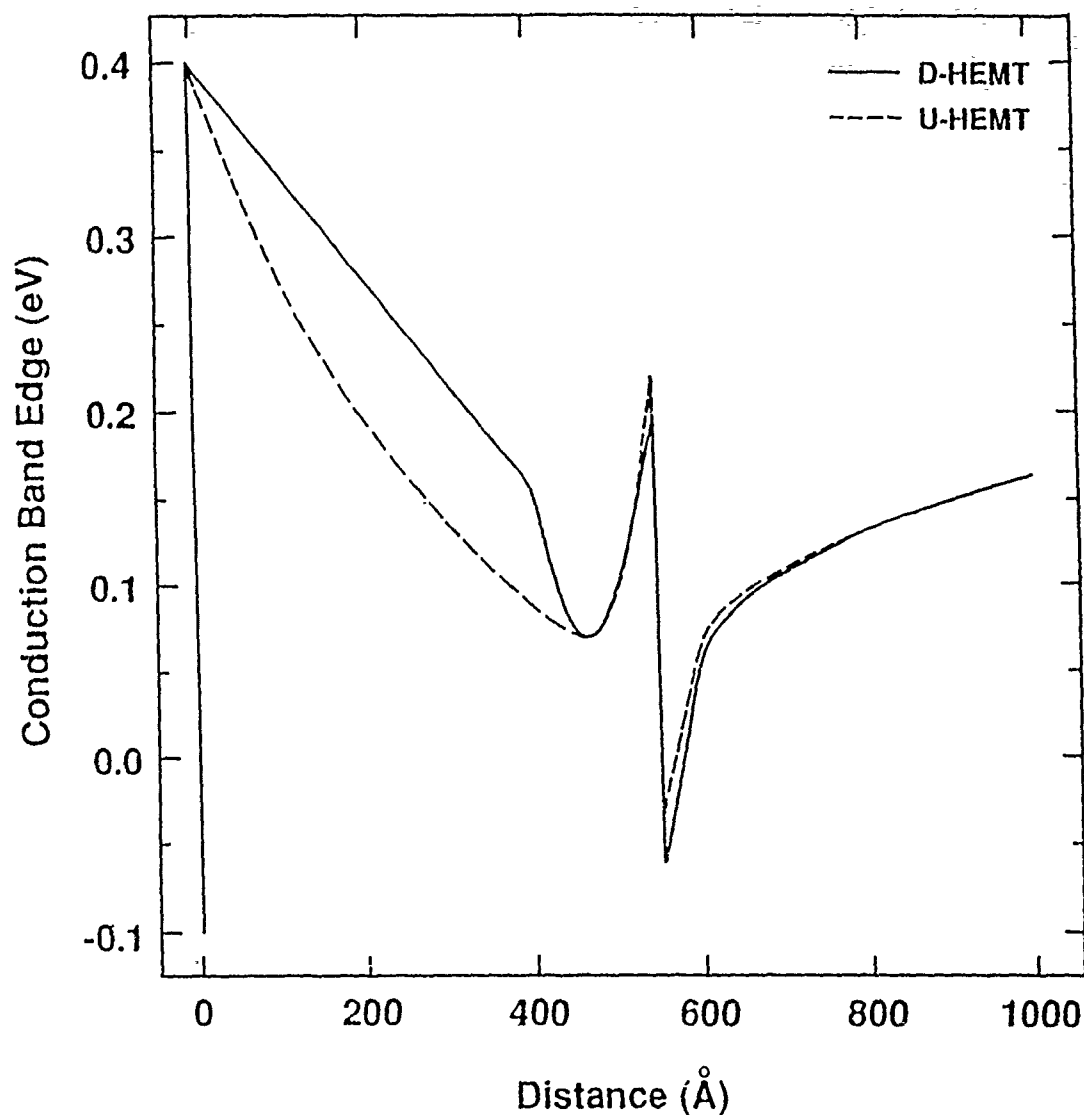


Figure 1: Cross-sectional view of conduction band profiles at $V_{gs} = 0.4$ V and $V_{ds} = 2.0$ V. The cross section is taken perpendicular to the middle of the $0.5 \mu\text{m}$ -long gate. The zero of the coordinate (i.e., 0 \AA) is chosen at the gate contact. An Al mole fraction of 0.3 and a Schottky barrier height of 0.8 eV are assumed for both the delta-doped HEMT (D-HEMT) and the uniformly doped HEMT (U-HEMT).

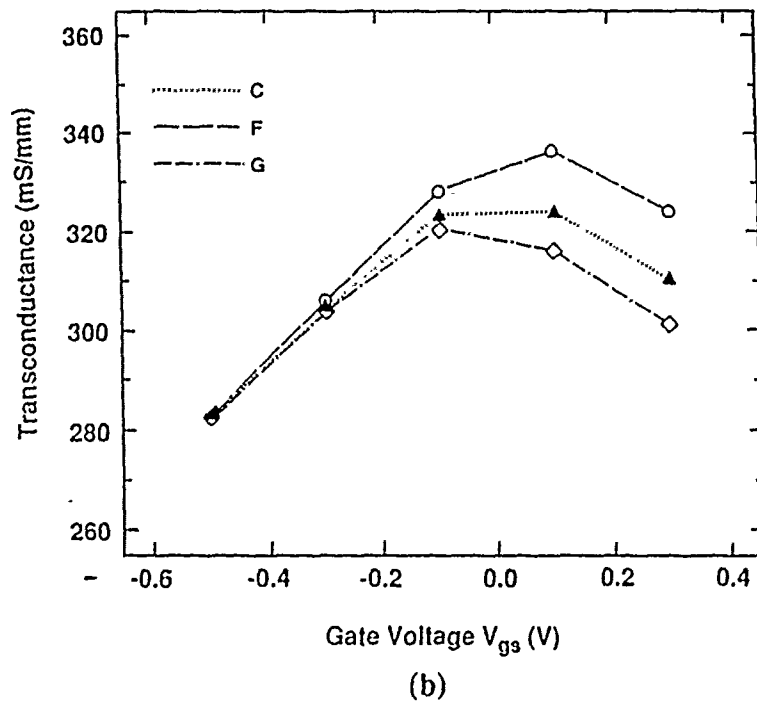
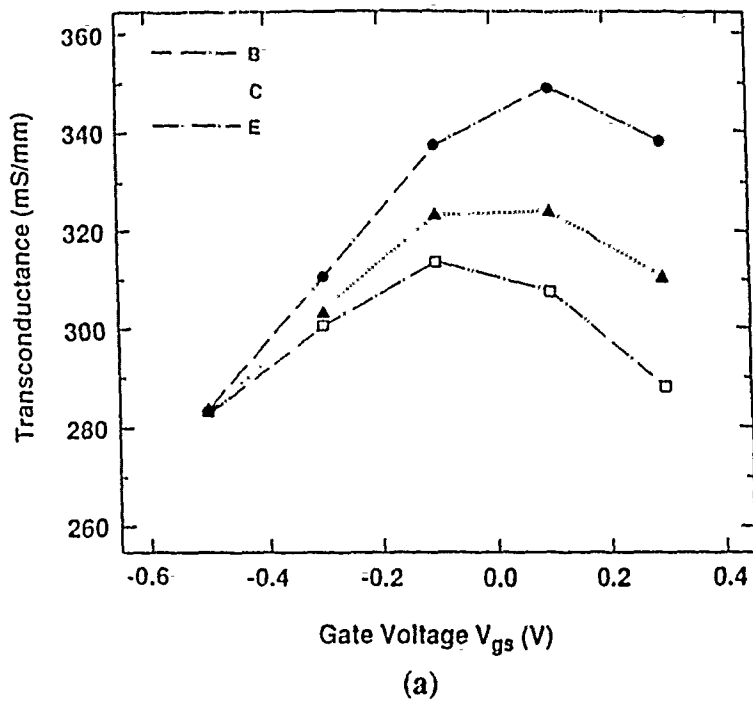


Figure 2: Transconductance as a function of gate-to-source bias V_{gs} at $V_{ds} = 2.0$ V in a $0.5\text{-}\mu\text{m}$ gate-length delta-doped HEMT: (a) For cases B, C, and E, the DX center concentration ratio varies from 0 (B) to 0.2 (C) to 1.0 (E) while the surface state density is fixed to $8.0 \times 10^{10} \text{ cm}^{-2}$. (b) For cases F, C, and G, the surface state density varies from 0 (F) to $8.0 \times 10^{10} \text{ cm}^{-2}$ (C) to $2.0 \times 10^{12} \text{ cm}^{-2}$ while the DX center concentration ratio is fixed to 0.2.

reduced parallel conduction, higher electron drift velocity and increased transconductance for the delta-doped HEMTs, especially at high (positive)-gate bias. We show in detail how band bending in the two structures changed the electron occupations in different layers within the devices (that is, top AlGaAs layer, channel layer, and substrate layer). Our simulation results also indicate that even though the delta-doped HEMT has less total AlGaAs doping than uniformly doped HEMT for the same threshold voltage and capacitance, performance improvement for delta-doped HEMTs can be realized due to the doping profile design. The advantage of delta-doped HEMTs over its uniformly doped counterparts in terms of high-channel electron density, reduced parallel conduction in AlGaAs layer, higher current and transconductance are clearly demonstrated in this study.

- Investigation of DX centers and surface states on delta-doped HEMTs — The roles of DX centers and surface states associated with doped AlGaAs layer are studied in this phase of our work. DX centers and surface states are believed to be the main mechanisms that degrade performances of HEMT structures. We studied delta-doped HEMTs under different defect situations (no defects, DX centers only, surface states only, and both DX center and surface states) under different bias conditions. We demonstrated that both DX centers and surface states indeed have negative effects on delta-doped HEMTs and provided physical explanations for the performance degradations. The analysis of bias dependence on the influences of the two defect levels indicates that the degrading effects are more significant with positive gate-to-source voltage. We found that the reasons for the degradation under the presence of DX centers and surface states are through reduced channel electron concentration, increased channel electron intervalley scattering, and enhanced real-space transfer. For the individual role of each defect state, we demonstrated that DX centers have more detrimental influence on drain current and transconductance than the surface states for delta-doped HEMTs (as shown in Fig. 2).
- Simulation of doping profile variation on delta-doped HEMT performance — Since the device improvements for delta-doped HEMTs result from the delta-doping, variation in the doping profile will play an important role on device performance optimization. We focused our study on the doping profile influence in this work. Various doping situations are studied. Specifically, we varied: a) the (AlGaAs) peak doping concentration and doping layer thickness (single delta-doped HEMTs) under constant threshold voltage conditions; and b) the spacing between two delta-doped layers for double delta-doped HEMT structures with identical total doping in the AlGaAs layer. Although the studied

double delta-doped HEMTs are experimentally unavailable, theoretical simulation of this device is both necessary and important to predict their performances and potential problems. Theoretical study of this new structure can provide valuable guidance for device design, fabrication, and characterization. In this work, device performances in terms of threshold voltage sensitivity, current drive, transconductance, cut-off frequency, and characteristic switching time are examined. Our simulation results show that: 1) For single delta-doped HEMTs with identical threshold voltages, the thinner the doped layer (with more heavily doped concentration), the better the overall device performance. 2) For double delta-doped HEMTs with an identical total doping in the AlGaAs layer, an increase in the spacing between two delta-doped layers leads to improved threshold voltage design but causes a slight degradation in transconductance, cut-off frequency, and switching time. As the gate bias increases, this degradation becomes less pronounced due to the higher "onset" of parallel conduction (for the structures with a larger spacing between the delta-doped layers).

(b) Analysis of Submicron Delta-Doped GaAs MESFETs

Efforts to achieve high speed and high frequency has led to continued efforts to develop novel device structures. One of the most promising structures is the MESFET which employs the delta-doping technique. Delta-doped GaAs MESFETs based on MBE and MOCVD materials have been investigated experimentally by several research groups. The results, while promising, show a wide diversity. The reported maximum transconductance for 0.5 μm channel-length delta-doped MESFETs, for example, range from 75 mS/mm to 400 mS/mm (as provided by both simulation and experimental device measurement in this work). Studies show that maximum intrinsic transconductance of the delta-doped MESFET is higher than that of comparable HEMT in the channel length range of 0.1 to 2.0 μm . Differences between experimental results and theoretical predictions may stem from material properties and processing conditions. On the other hand, design and optimization of such devices play an important role in the improvement of device performance. It is of practical importance to identify the key parameters for optimized device performances and to establish trade-offs needed for specific applications. It is obvious that a comprehensive study is required to investigate the influences of delta-doped MESFET parameters on performance and provide useful design guide.

In this work, we used a two-dimensional, drift-diffusion model to simulate the electrical characteristics of submicron delta-doped GaAs MESFETs. Poisson and electron current continuity equations were solved self-consistently and an analytical velocity-field relation which accounts for the velocity overshoot was employed. The results were compared with experimental measurements and showed very good agreement. Material parameters are based on the results

from delta-doped MBE materials provided by Dr. Bedair's group in the NCSU Electrical and Computer Engineering department. The device results were from DC measurement data provided by Texas Instruments based on the above materials. In this work, we studied the following issues:

- Delta-doping profile — We used a Gaussian distribution to approximate the actual doping concentration profile. Simulation of devices with 0.5 μm channel length gives very good agreement with fabricated experimental devices. For delta-doping profile simulation, we first simulated delta-doped MESFETs with different peak delta-doping concentrations and half width at half-maximum (HWHM) under constant threshold voltage; then the influence of the gate-to-channel distance was studied. We show that steeper doping profiles (i.e., high peak concentration and small HWHM of delta-doping) and a short gate-channel distance are preferred for improvement in transconductance. Current drive capability is increased for devices with steeper doping profile, but is decreased for devices with short gate-to-channel distance (due to the upward shift of threshold voltage as indicated by experimental results).
- Top layer background doping — We demonstrate in this work that a trade-off should be made in the design of the top layer background doping. Calculations show that significant increase in current drive ($\sim 200\%$) can be obtained at a low cost of slightly reduced transconductance ($\sim 10\%$) for devices using a relatively high top layer doping concentration (up to 20% of the peak delta-doping). The threshold voltage shift with respect to gate-to-channel distance for MESFETs with higher top layer background doping is considerably higher in absolute value but considerably lower in relative change when compared to a 'true' delta-doped device (with unintentional top layer background doping).
- Device lateral feature size — We performed scaling simulations for device lateral feature size. The result show that reducing the lateral features sizes (both channel length and source-to-drain spacing) brings improved transconductance, current drive capability, and cut-off frequency. For devices with identical channel length, a self-aligned structure is preferred in order to obtain minimum source-to-drain spacing. The improvement obtained by reducing the gate length is shown to be more profound than that achieved by reducing the source-to-drain spacing. Simulation results show that the main reason for the improvement is realized from an increase in average electron drift velocity along the device channel with reduced feature sizes.

2.2.5 Study of a Novel Heterojunction Real-Space Transfer Logic Transistor (RSTLT)

In this section, we report very preliminary results for a new heterojunction logic device. This device is called the real-space transfer logic transistor (RSTLT). These results will be presented at the International Electron Devices Meeting (IEDM) which will be held in Washington, DC, during December 8-11, 1991. The device structure consists of a GaAs channel which is sandwiched between two AlGaAs barrier layers. It has four-terminals for operation - a source, drain, and two collectors. The drain terminal is the signal input and the logic operation is provided at the two collectors. The basic structure realizes NOT and EQUIVALENT logic operations, and NAND/NOR operation can be achieved with two of the devices. A conservative estimate of the switching speed is approximately 3 psec total propagation delay. This estimate is based on self-consistent two-dimensional (ensemble) transient Monte Carlo simulations. The operation of the device is based on the principle that the spatial location for real-space transfer can be controlled by an input signal which steers current flow under one or both of the collector terminals. Thus, to perform logic operations, the carriers do not have to traverse the complete length of the channel. The principal speed limitation is determined by the rate of real-space transfer in the device.

The principles of operation and further discussion of device properties will be presented in a forthcoming paper.

2.3 Publications and Presentations

The funds for this program did not arrive at the University until March 1991. Thus, we have been working on the current contract for slightly more than seven months. However, during the last year we have made six oral presentations at national and international conferences. Also, twelve written manuscripts have been published in the refereed literature. In addition, six other manuscripts have been accepted for publication and five manuscripts have been submitted or are currently in preparation. The following paragraphs summarize the presentations and publications made under this program during the last year, and include material not previously reported to ONR in the last renewal proposal as well as material which was accepted for publication in 1990 and has since been published in 1991.

A. Conference Presentations and Seminars

K.W. Kim, M.A. Stroscio and J.C. Hall, "Frequencies of Confined Longitudinal-Optical Phonon Modes in Short-Period Strained Semiconductor Superlattices," presented at the SPIE International

Symposium on Optical and Optoelectronic Applied Science and Engineering, San Diego, CA, July 1990.

W.C. Koscielniak, M.A. Littlejohn and J.L. Pelouard, "Physical Speed Limits of Metal-Semiconductor-Metal Photodetectors," presented at the 17th International Symposium on Gallium Arsenide and Related Compounds, Jersey, Channel Islands, 24-27 September 1990.

M.A. Stroschio, K.W. Kim and M.A. Littlejohn, "Theory of Optical-Phonon Interactions in a Rectangular Quantum Wire," presented at the SPIE International Conference on Physical Concepts of Materials for Novel Optoelectronic Device Applications II: Device Physics and Applications, Aachen, Federal Republic of Germany, October 1990.

M.A. Stroschio, G.J. Iafrate, K.W. Kim, M.A. Littlejohn, H. Gronkin and G. Maracus. "Transition from LO-Phonon Scattering to SO-Phonon Scattering in Polar Semiconductor Superlattices," presented at the Workshop on Compound Semiconductor Microwave Materials and Devices, Fort Lauderdale, FL, February 1991.

M.A. Stroschio, K.W. Kim and Amit Bhatt, "Electron-Optical-Phonon Scattering Rates in Rectangular Quantum Wire," presented at the Annual March Meeting of the American Physical Society, St. Louis, MO, March 1991.

D.L. Woolard, R.J. Trew and M.A. Littlejohn, "Effect of Contacts on Transit Time and Velocity Overshoot in GaAs n^+-n-n^+ Structures," presented at the Workshop on Compound Semiconductor Microwave Materials and Devices, Fort Lauderdale, FL, February 1991.

(B) Refereed Publications, Papers Accepted for Publication and Papers Submitted or in Preparation

K.W. Kim, M.A. Stroschio, and J.C. Hall, "Frequencies of Confined Longitudinal-Optical Phonon Modes in Short-Period Strained Semiconductor Superlattices," *Proceedings of the SPIE International Symposium on Optical & Optoelectronic Applied Science and Engineering*, 1336, 43 (1990).

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M.A. Stroschio, K.W. Kim, M.A. Littlejohn and H. Chuang, "Polarization Eigenvectors of Surface-Optical Phonon Modes in a Rectangular Quantum Wire," *Phys. Rev. B*, 42, 1488 (1990).

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D.L. Woolard, H. Tian, R.J. Trew, M.A. Littlejohn and K.W. Kim, "A New Non-parabolic Hydrodynamic Model for Electron Transport in Semiconductors, accepted for publication in Phys. Rev. B.

H. Tian, K.W. Kim and M.A. Littlejohn, "An Investigation of Doping Profile Variations on AlGaAs/GaAs High Electron Mobility Transistor Performance," accepted for publication in J. Appl. Phys.

D.L. Woolard, R.J. Trew and M.A. Littlejohn, "Effect of Contact Regions on Transit Time and Velocity Overshoot in GaAs n^+-n-n^+ Structures, submitted to IEEE Trans. on Microwave Theory and Techniques.

D.L. Woolard, M.A. Littlejohn and R.J. Trew, "Impact of K-Space Transfer and Band Nonparabolicity on Velocity Overshoot in a GaAs Ballistic Diode," accepted for publication in Semicond. Sci. Technol.

K.W. Kim, M.A. Littlejohn, M.A. Strosio and G.J. Iafrate. "Transition from LO-Phonon to SO-Phonon Scattering in Mesoscale Structures," accepted for publication in Semicond. Sci. Technol.

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H. Tian, K.W. Kim, M.A. Littlejohn, S.M. Bedair and L. Witkowski, "Two-Dimensional Analysis of Short-Channel Delta-Doped GaAs MESFETs," submitted to IEEE Trans. on Electron Devices.

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W.C. Koscielniak, M.A. Littlejohn and J.L. Pelouard, "Performance Limitations of Metal-Semiconductor-Metal Photodetectors," to be submitted to the Journal of Optical and Quantum Electronics.

W.C. Koscielniak, M.A. Littlejohn and J.L. Pelouard, "Simulation of an InGaAs/InAlAs MSM Photodetector," to be submitted to Electronics Letters.

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4.0 PERSONNEL

Two faculty members in the Electrical and Computer Engineering Department at N.C. State University have been supported by this program. These faculty members are Dr. M.A. Littlejohn and Dr. K.W. Kim. Dr. Kim joined the NCSU faculty in August, 1988 after completing his Ph.D. degree at the University of Illinois under the direction of Prof. Karl Hess. We have also continued our strong interactions with Drs. M.A. Stroschio and G.J. Iafrate of the U.S. Army Research Office. These interactions are very important as our research moves more in the direction of quantum transport in mesoscopic systems. We are currently recruiting an additional Visiting Research Assistant Professor who will be involved in this research. In particular, we want to hire an individual with experience in band structure calculations who can contribute to our work in transport theory. Drs. Littlejohn and Kim serve as co-principal investigators on this research effort. Their resumes are given in Appendix C. They are responsible for day-to-day management and direction of the research program aspects. Three graduate students have been involved in this work and we plan to add a fourth student during the next spring who will pick up some of the work now being conducted by a Ph.D. student who began writing his doctoral dissertation this spring.

Appendix A

LIST OF REFEREED PUBLICATIONS ON THIS PROGRAM SINCE 1975

1. M. A. Littlejohn, J. R. Hauser, and T. H. Glisson, "Monte Carlo Calculation of Transport Properties of GaN", Appl. Phys. Letters 26, 625 (1975).
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Appendix B

This appendix contains the title page of each paper published in the refereed literature which were supported on the ONR project during the 1991 contract period. Copies of these papers have been sent to the program manager under separate cover. A list of these papers is included below.

K.W. Kim, M.A. Stroschio, and J.C. Hall, "Frequencies of Confined Longitudinal-Optical Phonon Modes in Short-Period Strained Semiconductor Superlattices," Proceedings of the SPIE International Symposium on Optical & Optoelectronic Applied Science and Engineering, **1336**, 43 (1990).

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Frequencies of confined longitudinal-optical
phonon modes in short-period
strained semiconductor superlattices

K. W. Kim
Department of Electrical and Computer Engineering
North Carolina State University
Raleigh, NC 27695-7111

Michael A. Strosio
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

J. C. Hall
Department of Electrical and Computer Engineering
North Carolina State University
Raleigh, NC 27709-2211

ABSTRACT

The theories describing the dispersion of longitudinal-optical (LO) phonon modes and electron--LO-phonon interactions are generalized to include the effects of both strain and confinement in semiconductor superlattices and semiconductor microstructures. In particular, the effects of strain and confinement on LO phonon frequencies are analyzed for short-period strained-layer superlattices as well as for semiconductor microstructures where effective force constants are altered near heterojunction interfaces.

1. INTRODUCTION

Confined phonons in semiconductor heterostructures have recently been the subject of both theoretical and experimental investigations. These efforts are due, in part, to the fact that scattering by the longitudinal-optical (LO) phonon modes is an important energy loss mechanism for a wide variety of III-V semiconductor devices.¹ Raman scattering measurements have been used to study the properties of phonon modes in quantum wells and superlattices.²⁻⁸ In particular, binary GaAs/AlAs superlattices have been experimentally investigated most extensively due to the simplicity in analysis (compared to ternary GaAs/AlGaAs superlattices) and the material familiarity.³⁻⁸ It is well known that phonon modes in the acoustic branch are propagative across the heterojunctions and, as a result, are "folded" into the reduced Brillouin zone,² while the modes in the optical branch are "localized" in each layer leading to descriptions of confined modes or slab modes.⁴ Furthermore, the localization of phonon modes near the heterojunctions leads to the well-known interface modes.⁵ In addition it is suggested that the Raman frequency shifts for confined LO-phonon modes can be used as a means to determine the bulk phonon dispersion relation (i.e., the equivalent wave-vector model)⁴ and as a probe to characterize the quality of interfaces.⁸ Frequency shifts due to confinement have been analyzed theoretically as well; the results obtained by a simple linear-chain model show a remarkable agreement with experimental data except in monolayer superlattices.³

VARIATION IN FREQUENCIES OF CONFINED LONGITUDINAL-OPTICAL PHONON MODES DUE TO CHANGES IN THE EFFECTIVE FORCE CONSTANTS NEAR HETEROJUNCTION INTERFACES

M. A. Sroscio,^(a) K. W. Kim,^(b) and J. C. Hall^(b)

^(a)U.S. Army Research Office
Research Triangle Park, NC 27709-2211

^(b)Department of Electrical and Computer Engineering
North Carolina State University
Raleigh, NC 27695-7911

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A linear-chain model with variable force constants for the couplings at heterojunctions is used to calculate the spectrum of confined longitudinal-optical (LO) phonon frequencies in a short-period strained-layer superlattice. Even for the case of a superlattice with only two atomic monolayers in each superlattice layer, it is demonstrated that the frequencies of confined LO-phonon modes are only weakly dependent on variations in interfacial force constants.

1. Introduction

Phonons in semiconductor heterostructures have received much attention. These efforts are due, in part, to the fact that scattering by the longitudinal-optical (LO) phonon modes is an important energy loss mechanism for electrons in a wide variety of III-V semiconductor devices.¹ In addition, Raman scattering measurements have been applied to study the properties of phonon modes in quantum wells and superlattices.²⁻⁸ Recently, Raman spectra have been used to characterize monolayer variations in the thicknesses of quantum wells.⁸ In the analysis and interpretation of Raman data for confined LO-phonon modes, it is convenient to model the confined LO modes as modes in a uniform isolated dielectric slab.⁸⁻¹¹ Such an approximate model is based on the assumption that atomic force constants at heterojunction interfaces are identical with those of the bulk or of uniform pseudomorphic layers. In this paper, the effect of varying force constants at the heterojunction interfaces of a strained-layer, short-period superlattice is analyzed by using a linear-chain model to determine the corresponding changes in the frequencies of the confined LO phonon modes. In the studies reported herein, a superlattice with only two atomic monolayers in each superlattice layer is modeled in order to determine the importance of perturbations in heterojunction interface force constants for a sys-

tem where such effects should be large. In particular, frequencies of confined LO-phonon modes are determined for a GaAs/GaP short-period superlattice with two monolayers per superlattice layer. It is found that varying interfacial force constants by values as extreme as 10% results in only about a 2% change in the frequencies of the confined LO-phonon modes. As a practical matter, changes in the frequencies of confined LO-phonon modes will generally be considerably less than 2% since in most superlattices and quantum wells the ratio of the number of bonds at interfaces to the number of bonds removed from interfaces is less than for the two-monolayer per layer case examined herein.

2. Linear-Chain Model with Variable Interfacial Force Constants

In order to introduce the basic properties of the linear-chain model used in this analysis, we will consider initially the case where interface effects are absent. Figure 1 depicts a schematic for the linear-chain system used to study the role of force-constant variations at heterojunction interfaces. The z axis is chosen as the growth direction of the lattice. Hence, for the longitudinal modes of interest, the atomic displacements are in the z direction. In the absence of strain, the force constant in each layer is estimated based on the frequencies of the

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DEVICE SIMULATION AUGMENTED BY THE MONTE CARLO METHOD*

M. A. Littlejohn[†], J. L. Pelouard^{††}, W. C. Koscielniak and D. L. Woolard
Electrical and Computer Engineering Department
North Carolina State University
Raleigh, NC 27695-7911

Abstract - This paper describes applications which combine Monte Carlo methods with other techniques to model semiconductor devices. These procedures can produce more effective means to describe the behavior of device structures requiring detailed physical descriptions and increased computational efficiency. Applications presented in this paper include: (a) simulation of transport across hetero-barriers with quasi-ballistic effects; (b) simulation of metal-semiconductor-metal photodetectors in which parasitic circuit effects are important; and (c) generation of transport parameters for use in drift-diffusion (and hydrodynamic) models while negating assumptions about the nature of the particle velocity distribution function.

1. Introduction

The Monte Carlo method is a versatile numerical technique for studying semiconductor materials and devices [1-4]. It provides mechanisms for including detailed physics of particle transport through solid state materials, especially the electron-phonon interaction and other scattering processes, realistic energy band structure, and temporal- and spatial-dependent parameters. Steady-state and transient properties are accessible with the Monte Carlo method. Realistic boundary conditions can be imposed which allow simulation of a variety of device structures. In principle, when coupled with a self-consistent numerical solver for Poisson's equation, the Monte Carlo method permits one to explore the properties of realistic two- and three-dimensional semiconductor devices with detail and precision. However, as more physical effects are included, as spatial dimensions decrease toward the quantum limit, and as fluctuation phenomena become more important, limitations to the Monte Carlo method become prohibitive for device simulations. In general, this limitation first manifests itself through requirements for increased computational resources and improved numerical algorithms.

The Monte Carlo method generates exact numerical solutions to the Boltzmann transport equation by stochastically tracking particle movements in phase space [2]. While use of numerical estimators yield parameters of physical interest (e.g., drift velocity), the fundamental quantity obtained from the simulation is the particle phase space distribution function. In this paper, we will discuss ways in which distribution function information obtained from Monte Carlo simulations can be used to augment the study of device behavior using other simulation methods.

2. Quasi-Ballistic Transport Across Hetero-Barriers

The distribution function experiences fundamental changes when an ensemble of carriers passes through an abrupt potential barrier. By imposing continuity of total particle energy and the parallel component of wave vector, there are two important consequences on the velocity distribution function. First, the normal component of the velocity vector is shifted to high positive values by an amount equal to the

A NEW NONPARABOLIC HYDRODYNAMIC MODEL WITH QUANTUM CORRECTIONS

D. L. Woolard^(a), M. A. Strosio^(b), M. A. Littlejohn^(a,b),
R. J. Trew^(a) and H. L. Grubin^(c)

^(a)Electrical and Computer Engineering Department
North Carolina State University
Raleigh, North Carolina 27695-7911

^(b)U.S. Army Research Office
Research Triangle Park, North Carolina 27709

^(c)Scientific Research Associates Inc.
Glastonbury, Connecticut, 06033-6058

Abstract - This paper presents a new hydrodynamic transport model with non-parabolic conduction bands and quantum correction terms. For the first time solutions for the full quantum balance equations, applied to an ultrasmall electron device, are presented.

1. Introduction

Requirements for faster electronics have produced smaller devices influenced by quantum interference effects which can not be modeled by classical theory. These devices operate under nonequilibrium conditions where the average carrier energy reaches many times its equilibrium value. To address these problems several approaches [1] have been considered. This paper describes a preliminary investigation into solutions for electron density, average velocity and average energy for an ultrasmall electronic structure under the conditions of nonclassical electron transport, using an approach previously described as quantum hydrodynamics [2].

2. The Nonparabolic Model

First, we present a brief summary of a unique form of the hydrodynamic transport model applicable to nonparabolic conduction bands. A complete description of this model will be formalized elsewhere [3]. Our hydrodynamic model was developed by studying moments of the Boltzmann transport equation [4]. This process was achieved using the moment operators $\Psi_1 = 1$, $\Psi_2 = u(k) = \frac{\hbar k}{m(k)}$, and $\Psi_3 = \frac{1}{2}m(k)u(k) \cdot u(k) \approx E_c(k)$. Here, the Kane dispersion relation, $\frac{\hbar^2 k^2}{2m^*} = E_c(k) + \alpha E_c$, has been used to define $u(k)$ and $m(k) = m^* \sqrt{1 + \frac{2\alpha \hbar^2 k^2}{m^*}}$. These moment operators were chosen because they lead to a form which can be manipulated more easily and one in which simplifying approximations can be seen more clearly. Performing the moment process and simplifying to first order yields immediately the

Physical speed limits of metal-semiconductor-metal photodetectors

W. C. Koscielniak, M. A. Littlejohn and J.-L. Pelouard*
Department of Electrical and Computer Engineering
North Carolina State University
Raleigh, NC 27695-7911 USA

Metal-semiconductor-metal (MSM) photodetectors are of interest for integrated optoelectronic circuits (OEICs) and other discrete circuit applications because this very high-speed device can be fabricated using conventional GaAs integrated circuit technology. The typical configuration of such a photodetector consists of two interdigitated Schottky electrodes patterned on the semiconductor surface. The fastest MSM detector has an intrinsic bandwidth of 105 GHz, which compares well with bandwidths of other Schottky photodiodes. The potential to achieve even larger bandwidths appears to be quite promising.

We have performed simulations of intrinsic detectors and obtained time responses for devices with interfinger spacings between 0.1-1 μm . A self-consistent ensemble Monte Carlo simulation method was employed to study electron and hole transport under low illumination intensity. The Monte Carlo method provides mechanisms for including detailed physics of carrier transport, especially the electron-phonon interaction and other scattering processes, realistic energy band structure, and temporal- and spatial-dependent parameters. Realistic boundary conditions are imposed and the utilization of a self-consistent numerical solver for Poisson's equation permits us to simulate realistic one- and two-dimensional structures with detail and precision. In addition, the time-dependent Schrödinger equation is solved for the detector with 0.1 μm distance between fingers under an assumption of collisionless carrier transport, and a comparison between the two different methods is made. The devices are dominated by stationary hot electron and hole transport.

A parasitic circuit is introduced to more closely model realistic devices. The intrinsic responses are used in a circuit simulator to obtain the time responses of photodetectors due to excitation by a very short optical pulse. The spectral power density is calculated using a fast Fourier transform (FFT) to predict the bandwidth of intrinsic and extrinsic photodetectors. This simulation technique is shown to yield good agreement with published experimental data for a GaAs photodetector.

For GaAs MSM photodetectors, we predict that bandwidths in excess of 150 GHz can be achieved for devices with 0.1-0.2 μm interfinger spacing. The parasitic effects of the contact pattern are critical in the performance of such short devices, and further optimization of the interfinger coplanar transmission line could result in even higher bandwidths. The role of the transient response of holes on the intrinsic and extrinsic photodetector response and bandwidth will be discussed. Results are also presented for InAlAs/InGaAs/InP MSM photodetectors. These devices operate at longer wavelengths than GaAs MSM photodetectors, and are thought to provide potential for high-speed near-infrared transceivers. Our results predict that hole transport and transient response limit the bandwidth achievable with this material system to about 25 GHz for MSM photodetectors with 0.2 μm interfinger spacing and current contact design geometries.

* Current Address: Laboratoire de Microstructures et de Microélectronique (CNRS), 196 Ave Henri Ravéra, 92220 Bagneux, France.

Polarization eigenvectors of surface-optical phonon modes in a rectangular quantum wire

Michael A. Stroscio

U.S. Army Research Office, P.O. Box 12211, Research Triangle Park, North Carolina 27709-2211

K. W. Kim and Michael A. Littlejohn

Department of Electrical and Computer Engineering, North Carolina State University, Raleigh, North Carolina 27695-7911

Hsuhung Chuang

Department of Electrical Engineering, Duke University, Durham, North Carolina 27706

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The polarization eigenvectors and dispersion relations for confined longitudinal-optical (LO) and surface-optical (SO) phonon modes in a rectangular quantum wire are derived within the continuum approximation. The SO and confined LO modes are compared for a quantum wire with a square cross section in the limit of a vanishing phonon wave vector along the quantum-wire axis. For this case, it is demonstrated that the SO mode becomes dominant over the confined LO modes in interaction with electrons and must be taken into account in calculating the electron-optical-phonon scattering rate.

Epitaxial techniques for the growth of compound-semiconductor structures have advanced to the level where it is possible to fabricate wire-like regions of low-band-gap semiconductor material surrounded completely by regions of higher-band-gap semiconductor material. In particular, such wire-like structures have been realized with rectangular cross sections having small dimensions relative to the thermal de Broglie wavelength.¹ In these structures the electron-optical-phonon scattering rate is affected not only by changes in the electron wave function due to the confining rectangular potential but also by changes in the longitudinal-optical (LO) phonon modes caused by phonon confinement. Fasol *et al.*² have recently presented striking experimental evidence of phonon confinement. Size effects on the total scattering rates for polar-optical-phonon scattering of one-dimensional (1D) electron gases in quantum wires and two-dimensional (2D) electron gases in quantum wells have been evaluated previously by Leburton.³ Recently, Leburton's treatment of 1D electron-LO-phonon scattering was extended by replacing bulk LO-phonon modes with the confined LO-modes of a quantum wire.⁴ The scattering rate calculations of Ref. 4 included confined LO-phonon modes of a rectangular wire and neglected electron scattering due to the surface-optical (SO) phonon modes at the quantum-wire boundaries. In this Rapid Communication, the confined LO- and SO-phonon modes are derived for a rectangular quantum wire. In the limit of small (phonon) wave vectors along the quantum-wire axis, it is shown that the contribution of electron-SO-phonon scattering to the ground-state electron-LO-phonon scattering rate becomes significant and cannot be neglected compared to the contribution by the confined LO-phonon modes.

Since the early work of Fuchs and Kliever,^{5,6} the effects of confinement on LO-phonon modes have been studied theoretically by a number of authors for the case of phonon confinement in a quantum well.⁷⁻⁹ Only re-

cently have confined LO-phonon modes been studied in more complex structures such as quantum wires⁴ and strained-layer short-period superlattices.^{10,11} In this study, the polarization eigenvectors for the confined LO-phonon and the SO-phonon modes of a quantum wire surrounded by a medium with unity dielectric constant are derived in the continuum approximation.^{4,5,7-9} For phonon wavelengths long compared with the lattice constant, continuum models are expected to be valid^{5,7,9} and the results of such models agree well with those of microscopic models.¹² The quantum wire is taken to have a dielectric constant ϵ_2 , and to be bounded by $\pm L_x/2$ and $\pm L_z/2$ in the y and z directions, respectively. The region surrounding the quantum wire is taken to have a dielectric constant ϵ_1 ($=1$). The confined LO-phonon modes for such a quantum wire have been given previously.⁴

Since this system is translationally invariant in the x direction, the potential describing the optical-phonon modes may be taken as

$$\Phi(\mathbf{r}) = \Phi(y, z)e^{ik_x x}, \quad (1)$$

where k_x is the phonon wave vector in the x direction. In the absence of any free charge, the divergence of the displacement vector must vanish and it follows that the potential $\Phi(y, z)$ of the phonon modes must satisfy

$$\epsilon \left\{ \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} - k_x^2 \right\} \Phi(y, z) = 0, \quad (2)$$

where $\epsilon = \epsilon_2$ for $-L_x/2 < y < +L_x/2$ and $-L_z/2 < z < +L_z/2$, outside of this region which defines the quantum wire, $\epsilon = \epsilon_1$. The derivation of Eq. (2) is straightforward upon taking $\mathbf{E}(\mathbf{r}) = -\nabla\Phi(\mathbf{r})$, $\mathbf{D}(\mathbf{r}) = \epsilon\mathbf{E}(\mathbf{r}) = \mathbf{E}'(\mathbf{r}) + 4\pi\mathbf{P}(\mathbf{r})$, and $\Phi(\mathbf{r})$ as given by Eq. (1), a similar treat-

Influence of DX centers and surface states on δ -doped high-electron-mobility transistor performance

H. Tian, K. W. Kim, and M. A. Littlejohn

Department of Electrical and Computer Engineering, North Carolina State University, Raleigh, North Carolina 27695-7911

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The roles of DX centers and surface states associated with the n -AlGaAs layer of δ -doped AlGaAs/GaAs high-electron-mobility transistors have been investigated by employing a two-dimensional, self-consistent ensemble Monte Carlo simulation. It is found that both DX centers and surface states degrade device performance, particularly as gate-to-source voltage increases. This degradation is manifested largely through reduced channel electron concentration, increased intervalley scattering, and enhanced real-space transfer. Of the two defect states, DX centers have more detrimental influence on drain current and transconductance.

I. INTRODUCTION

Recent studies¹⁻⁴ of the AlGaAs/GaAs high-electron-mobility transistor (HEMT) have indicated that deep donor levels (DX centers) and surface states associated with the n -AlGaAs layer can degrade device performance significantly. Experimental measurements show that there is a sharp increase in the concentration of trapped carriers by DX centers (and a subsequent collapse in device transconductance) in the $\text{Al}_x\text{Ga}_{1-x}\text{As}$ layer with Al mole fraction $x > 0.2$. Similar degradation has been observed in connection with surface states as well. The nature of DX centers in AlGaAs has been a subject of controversy, investigated by many authors experimentally.⁵⁻⁷ Mizuta *et al.*⁵ describe the DX center as a simple substitutional donor, while the work by Dhar *et al.*⁶ reveals that there are two closely spaced deep donor levels in addition to a shallow donor level. Study also shows that the ratio of shallow donor density to deep donor density exhibits substantial variations from sample to sample, depending upon the material composition and (possibly) some other growth parameters.

To date, theoretical investigations^{4,8,9} of the effects of DX centers and surface states on device performance have been scarce and largely inconclusive. In particular, most of the efforts have been devoted to the phenomenological description (i.e., parameter fitting) of device degradation in the presence of either DX centers or surface states, rather than to physical models which can elucidate the underlying mechanisms. The combined trapping effects by both DX centers and surface states have not been identified and, in addition, are not well understood.

It is the purpose of this paper to present results of our study on the influence of DX centers and surface states employing a realistic, physical model. The δ -doped AlGaAs/GaAs HEMT has been chosen as a specific structure to be studied due to its superior performance and recent interest compared to the uniformly doped counterpart.¹⁰⁻¹³ The collective roles of DX centers and surface states are examined for 0.5- μm gate-length δ -doped AlGaAs/GaAs HEMTs with general trapping situations

and different bias conditions by employing a two-dimensional, self-consistent ensemble Monte Carlo simulation. The results clearly indicate the importance of DX centers and surface states on device modeling and provide an explanation for detailed degradation mechanisms.

II. MODEL

The Monte Carlo model incorporates three-valley (Γ - L - X) nonparabolic analytical band structures for both AlGaAs and GaAs. The trajectories of about 1.5×10^4 sample electrons are traced both in real space and in momentum space under the influence of a two-dimensional electric field generated by a self-consistent Poisson equation solver. These electrons are subject to relevant scattering mechanisms such as polar optical, intervalley, ionized-impurity, and electron-electron scatterings. The contribution by the collective excitations of the electron gas (i.e., plasmon) is considered through frequent updating of the electric-field profile (every 2×10^{-15} s). Real-space transfer of electrons between GaAs and AlGaAs is included. Since the two-dimensional quantum effects are relatively unimportant for the electrons in the high-field region,¹⁴ we treat the AlGaAs/GaAs interface potential classically and ignore size quantization. The effect of carrier degeneracy is taken into account for electrons in the Γ valley by employing Fermi statistics with the calculated local quasi-Fermi level and Γ -valley average electron energy.^{11,15} Charge neutrality in a small region adjacent to the source and drain contacts is maintained throughout the simulation and serves as the criterion for electron injection. Figure 1 shows a schematic drawing of a typical 0.5- μm δ -doped AlGaAs/GaAs HEMT structure studied in this paper. The device consists of a 400-Å unintentionally doped ($5 \times 10^{14} \text{ cm}^{-3}$) top AlGaAs layer, a 100-Å step-doped ($5 \times 10^{18} \text{ cm}^{-3}$) n^+ -AlGaAs layer, and a 50 Å unintentionally doped ($5 \times 10^{14} \text{ cm}^{-3}$) AlGaAs spacer layer followed by a 2000-Å unintentionally doped ($5 \times 10^{14} \text{ cm}^{-3}$) GaAs layer. The contact doping is assumed to be $1 \times 10^{18} \text{ cm}^{-3}$. An Al mole fraction of 0.3 is used for each AlGaAs layer. The gate-electrode Schottky bar-

Theory of optical-phonon interactions in a rectangular quantum wire

Michael A. Stroscio
U.S. Army Research Office
P. O. Box 12211
Research Triangle Park, North Carolina 27709-2211

K. W. Kim and M. A. Littlejohn
Department of Electrical and Computer Engineering
North Carolina State University
Raleigh, North Carolina 27695-7911

ABSTRACT

The Hamiltonian describing the interaction of both confined longitudinal-optical and surface-optical phonons with charge carriers is derived from the macroscopic dielectric continuum model for the case of a rectangular quantum wire where phonon confinement occurs in two of the three spatial dimensions. The full interaction Hamiltonian is used to calculate the total scattering rate for electron-optical-phonon scattering of electrons traversing a GaAs square quantum wire. The results demonstrate that the interaction by the surface-optical phonon modes is very strong and may dominate over other scattering processes, especially with dimensions of about 100 Å or less. A considerable decrease in the total scattering rate for optical phonons as a result of simple reduction in dimensionality is not observed in this study.

1. INTRODUCTION

Epitaxial techniques for the growth of compound-semiconductor structures have advanced to the level where it is possible to fabricate wire-like regions of narrow-band-gap semiconductor material surrounded completely by regions of large-band-gap semiconductor material. In particular, such wire-like structures have been fabricated with rectangular cross sections having dimensions small relative to the electron thermal de Broglie wavelength; furthermore, optical anisotropy measurements on these wire-like structures provide evidence of two-dimensional quantum confinement of charge carriers.¹ In such structures, the electron-optical-phonon scattering rate is affected by changes in the wave functions of the charge carriers due to the confining rectangular potential but also by changes in the carrier-optical-phonon interaction Hamiltonian caused by phonon confinement and localization of charge carriers due to the confining rectangular potential. Indeed, recent measurements on cylindrical quantum wires² have provided striking evidence of surface-optical (SO) modes and Fasol et al.³ have experimentally verified phonon confinement. The effects of carrier confinement on the total scattering rates for polar-optical-phonon scattering in quantum wells and quantum wires have been evaluated previously by Leburton⁴ with bulk longitudinal-optical (LO) phonon modes.

In this paper, one-dimensional (1D) electron-optical-phonon scattering rates in rectangular quantum wires are determined by including the effects of carrier confinement as well as by replacing the bulk LO-phonon modes by the confined LO-phonon modes and surface-optical (SO) phonon modes for a rectangular quantum wire. While optical-phonon confinement effects are clearly evident in quantum-well structures,³ the results of this paper demonstrate that carrier-optical-phonon scattering may dominate over other

Analysis of Delta-Doped and Uniformly Doped AlGaAs/GaAs HEMT's by Ensemble Monte Carlo Simulations

Ki Wook Kim, *Member, IEEE*, Hong Tian, and Michael A. Littlejohn, *Senior Member, IEEE*

Abstract—Transport properties and device performance of delta-doped and uniformly doped AlGaAs/GaAs high electron mobility transistors (HEMT's) with identical threshold voltages and gate capacitors are investigated with two-dimensional, self-consistent ensemble Monte Carlo simulations. The model includes the effects of real-space transfer and carrier degeneracy, as well as the influence of DX centers and surface states. A one-to-one comparison of simulation results for the two devices demonstrates superior performance for the delta-doped HEMT and provides physical basis for the observed improvements. In particular, the delta-doped HEMT maintains its superior device performance as gate bias is increased. The simulations provide reasons for these improvements. The predicted advantages of the delta-doped HEMT include high channel electron density and high channel drift velocity, which stem primarily from improved channel electron confinement, reduced parallel conduction at high gate-to-source voltage, and reduced peak channel electric field. These advantages of delta-doped HEMT are manifested in higher transconductance and improved drain current drive capability at a wider gate-to-source voltage, which are desirable properties for ultra-fast digital and microwave device applications.

I. INTRODUCTION

THE HIGH electron mobility transistor (HEMT) is a promising candidate for ultra-fast digital and microwave device applications. Conventional uniformly doped AlGaAs/GaAs HEMT's are superior to comparable MESFET structures in overall device performance. However, further device improvement is limited by the occurrence of persistent photoconductivity [1], threshold-voltage shift [2], and collapse of I - V characteristics [3] due to effects of deep donors in the AlGaAs layer. The utilization of low Al mole fraction can reduce these effects; however, this also reduces the conduction-band-edge discontinuity, resulting in decreased channel electron density. This inherent limitation can be circumvented either by device structure modifications (such as delta-doping [4]–[8]) or by using pseudomorphic heterostructures [9], [10]. Recently, much attention has been paid to delta-

doped (also referred to as pulse-doped [4], [5] or planar-doped [7]) HEMT structures due to the maturity of epitaxial technology and excellent lattice match for the AlGaAs/GaAs system. By introducing an unintentionally doped i -layer between Schottky gate and n^+ -AlGaAs layer, the delta-doped HEMT's provide high channel electron density, reduced trapping effect, and improved threshold voltage control as well as high breakdown characteristics. Also, one expects improved current drive capability and high transconductance due to high electron density and small gate-to-channel spacing for such devices.

Although the advantages of the delta-doped HEMT over the uniformly doped HEMT have been shown experimentally, detailed theoretical investigations are essential to fully understand underlying physics and exploit advantages of delta-doping on electron transport and device performance in the submicrometer regime. While systematic analysis of conventional uniformly doped AlGaAs/GaAs HEMT's and pseudomorphic HEMT's have been reported by many authors [11]–[14], such studies on delta-doped structures have been rare and mainly first-order [7], [8]. It is well known that the operation of submicrometer heterostructure devices involves highly nonlinear transport, such as hot-electron effects and real-space transfer, and requires a powerful device model to accurately describe carrier transport behavior and device performance. One of the most sophisticated and complete tools is the ensemble Monte Carlo simulation coupled with a self-consistent Poisson solver. In this study, we examine the transport properties and device performance of comparable 0.5- μm gate-length delta-doped HEMT and uniformly doped HEMT (hereafter, D-HEMT and U-HEMT, respectively) using a self-consistent two-dimensional ensemble Monte Carlo simulation. Our simulation results demonstrate the superior performances of D-HEMT's to those of comparable U-HEMT's in terms of device structure, doping, and bias conditions and provide a clear physical explanation for the improvements.

II. MODEL

The AlGaAs/GaAs HEMT structure used in the simulations is illustrated in Fig. 1. For the D-HEMT, the device consists of a 400-Å unintentionally doped ($5 \times$

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The authors are with the Department of Electrical and Computer Engineering, North Carolina State University, Raleigh, NC 27695-7911.
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Constraints on the polar-optical-phonon influence functional in heterostructures

Leonard F. Register

*Electrical and Computer Engineering Department, North Carolina State University, Raleigh, North Carolina 27695-7911
and Beckman Institute and Coordinated Science Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801*

Michael A. Strosio

U.S. Army Research Office, Research Triangle Park, North Carolina 27709

Michael A. Littlejohn

*Electrical and Computer Engineering Department, North Carolina State University, Raleigh, North Carolina 27695-7911
and U.S. Army Research Office, Research Triangle Park, North Carolina 27709*

(Received 17 December 1990; revised manuscript received 4 March 1991)

The Feynman influence functional for the polar coupling of carriers to confined phonon modes in heterostructures is considered. It is found that the partial contributions to the total influence functional from the individual branches of the optical-phonon energy spectrum are related and constrained by conservation relations. The derivation of these conservation relations requires no specific functional form for the phonon modes; rather it employs only the inherent orthogonality and mathematical completeness of the classical vibrational modes over the crystal-lattice degrees of freedom. In the bulk-crystal limit these conservation relations lead to the familiar results of Feynman; for arbitrary heterostructures, these conservation relations provide a basis for an estimation of the influence functional from limited knowledge of the spatial confinement of the individual phonon branches.

I. INTRODUCTION

The Feynman path-integral (FPI) formulation of quantum mechanics allows formal inclusion of carrier-phonon coupling to all orders in the coupling potential via the influence functional.^{1,2} For this reason, the FPI formalism long has been used to calculate carrier self-energies and effective masses in bulk semiconductors.³⁻⁶ More recently, the FPI formalism has been extended to the study of confined carriers in ultrasmall heterostructure geometries,⁷ including recent advances in numerical methods.⁸⁻¹⁰ However, in heterostructures, beyond the confinement of carriers, the confinement of phonons should be considered as well. Here, this latter confinement effect on the influence functionals for polar coupling of carriers to longitudinal-optical (LO) phonons is considered, without assuming any specific functional form for the phonon modes. In Sec. II, the influence functional is defined in terms of the carrier-phonon interaction Hamiltonian. In Sec. III, it is shown that the partial contributions to the total influence functional from the individual branches of the LO-phonon spectrum are related and constrained by conservation relations. In Sec. IV, it is shown that these conservation relations lead

to the familiar results of Feynman^{3,4} in the bulk-crystal limit, and that for heterostructures they provide a basis for estimation of the influence functional from limited knowledge of the spatial confinement of the individual phonon branches.

II. PATH-INTEGRAL FORMALISM

Consider a coupled carrier-phonon system with quantum-mechanical Hamiltonian of the form

$$H = -\frac{\hbar^2}{2m^*} \nabla_r^2 + V(r) + \sum_m \left[-\frac{\hbar^2}{2} \frac{d^2}{d\xi_m^2} + \omega_m^2 \xi_m^2 + \phi_m(r) \xi_m \right], \quad (1)$$

where r is the carrier coordinate, ξ_m are the phonon coordinates, $\hbar\omega_m$ are the uncoupled phonon energies, and $\phi_m(r)$ are real functions characterizing the carrier position dependence in the carrier-phonon interaction. For this system, the equilibrium density matrix for the carrier averaged over the phonon coordinates and subject to a Maxwell-Boltzmann distribution in energies at temperature T is given by

$$\rho(r, r'; T) = \int_{r'}^r \exp \left[-\frac{1}{\hbar} \int_0^{\hbar/\hbar_B T} \left[\frac{1}{2} m^* |\dot{r}(t)|^2 + V(r(t)) \right] dt \right] \mathcal{F}[r(t)] \mathcal{D}r(t) \quad (2)$$

in the FPI formalism.² Here, " $\int_{r'}^r \cdots \mathcal{D}r(t)$ " signifies an integral over all paths from r' to r that are continuous functions of time, and $\mathcal{F}[r(t)]$ is the influence functional. $\mathcal{F}[r(t)]$ accounts for coupling between the carriers and phonons to all orders in the coupling potential and is given by⁴

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The Application of Monte Carlo Techniques in Advanced Hydrodynamic Transport Models

D. L. Woolard, H. Tian, M.A. Littlejohn, R. J. Trew, and K.W. Kim

Electrical and Computer Engineering Department
North Carolina State University
Raleigh, North Carolina 27695-7911

1 Introduction

The Monte Carlo method is a powerful technique for investigating electron transport physics in semiconductors and semiconductor devices[1, 2, 3]. Monte Carlo is a general statistical numerical method for solving mathematical and physical problems which was firmly established long before being introduced to semiconductor physics[4]. In the case of electron transport, the method provides the most efficiently implemented and physically adaptive technique currently available to determine *exact numerical* solutions of the electron motion in semiconducting materials and devices[5, and references therein].

The Monte Carlo method provides a relatively simple and accurate indirect approach to determine particle distribution functions and transport parameters resulting from the Boltzmann transport equation subject to complex scattering mechanisms[6, 7]. In the method, a type of mathematical experiment is performed where the trajectory of an electron (or an ensemble of electrons) is simulated subject to applied fields and given scattering mechanisms. The duration of the carrier free flights and the particular collision events are selected stochastically (randomly) according to known scattering probabilities which describe the microscopic processes. When an electron is tracked over a *sufficiently long* history the dynamics can then be used to estimate time-independent properties of the entire electron gas (For time and/or space dependent problems, the sample ensemble must be sufficiently large to accurately represent the entire electron gas). This procedure permits the investigation and interpretation of physical phenomena unattainable solely by experimental methods. Thus, the Monte Carlo method is extremely valuable to solid state physics from both a theoretical and experimental point of view.

Transition from longitudinal-optical phonon scattering to surface-optical phonon scattering in polar semiconductor superlattices

Michael A. Stroscio and Gerald J. Iafrate

U.S. Army Research Office, Research Triangle Park, North Carolina 27709-2211

K. W. Kim and M. A. Littlejohn

Department of Electrical and Computer Engineering,

North Carolina State University, Raleigh, North Carolina 27695-7911

Herbert Goronkin

Motorola Phoenix Corporate Research Laboratory, Tempe, Arizona 85284

George N. Maracas

Department of Electrical Engineering, Arizona State University, Tempe, Arizona 85281

(Received 11 March 1991; accepted for publication 31 May 1991)

Dielectric continuum models of optical-phonon modes predict an enhancement in the strength of the surface-optical (SO) modes in double-barrier heterostructures as the heterojunction-to-heterojunction separation is reduced. There is currently no consensus on the nature of the electron-SO-phonon coupling interaction. In this work, the ratio of electron scattering by the SO-phonon modes to that by the confined longitudinal-optical (LO) phonon modes is calculated for a GaAs/AlAs short-period superlattice based on the assumption that the electron-SO-phonon interaction may be described by a scalar potential. The scaling of the ratio of electron-SO-phonon scattering to electron-LO-phonon scattering as a function of the superlattice period provides a sensitive test of the appropriateness of the scalar-potential model.

Electron interactions with longitudinal-optical (LO) phonon modes in heterostructures are strongly affected by the changes in the Fröhlich Hamiltonian caused by phonon confinement and localization, as well as by the changes in the electronic wave function due to the confining potential. The presence of heterointerfaces gives rise to the confinement of optical phonons in each layer (i.e., confined mode) and the localization in the vicinity of interfaces [i.e., interface mode or surface-optical (SO) mode]. There have been suggestions that interactions by the interface modes can be significant and that the scattering rate due to the confined modes can be considerably reduced in some structures compared to the bulk LO-phonon scattering rate.¹⁻³ Therefore, an appropriate treatment of the optical-phonon modes in quantized systems is essential for the understanding of electron transport in heterostructures. Recently, both macroscopic and microscopic approaches to electron-optical-phonon interactions in heterostructures¹⁻¹¹ have been applied in theoretical treatments. Enhanced electron-SO-phonon (i.e., electron-interface-phonon) scattering in polar semiconductors with confining dimensions less than about 50 Å has been indicated recently^{12,13} on the basis of a scalar-potential model. The appropriateness of using a scalar potential to model the electron-SO-phonon interaction has been questioned.¹⁴ In this letter, we model the electron-SO-phonon interaction with a scalar potential to calculate the ratio of electron-SO-phonon scattering to electron-confined-LO-phonon scattering in a short-period GaAs/AlAs superlattice. The results provide a criterion which, in conjunction with experiments, can be used to examine the validity of the scalar-potential model.

A GaAs/AlAs short-period superlattice is considered

in this study. Each GaAs layer has width a and each AlAs has width b . We will consider the case where a uniform electron current J is incident parallel to the superlattice heterojunctions. The ratio of electron-SO-phonon scattering to electron-LO-phonon scattering in the GaAs/AlAs superlattice is calculated through the Fermi golden rule by treating the electron-LO-phonon and electron-SO-phonon interaction Hamiltonians^{4,6} as perturbation Hamiltonians and by taking the electronic wave function in the z direction as that given by Cho and Prucnal for the maximum edge of the first subband;¹⁵ that is,

$$|k_z = D\rangle = \frac{e^{ik_y r}}{\sqrt{L^2}} \left(\frac{2}{a+b} \right)^{1/2} \cos\left(\frac{\pi z}{a+b} \right), \quad (1)$$

where k_{\parallel} is the electron wave vector parallel to the superlattice heterojunctions, L^2 is the heterojunction area (under the assumption that $L \gg a + b$ and $L \rightarrow \infty$), r defines the parallel components of the position vectors in the superlattices, and the other quantities are as discussed above. The origin of the z axis (i.e., growth direction) is chosen at the middle of a GaAs layer. Taking the electron-optical-phonon interaction Hamiltonians to be as in Ref. 6, the matrix elements for the emission of the lowest order confined LO phonons and the $S \pm$ symmetric phonons are given, respectively, by

$$M_{C(S \pm)} = \langle k', N_q + 1 | H_{C(S \pm)} | k, N_q \rangle, \quad (2)$$

where N_q is the phonon occupation number and k' is the electron wave vector after phonon emission. Performing the indicated overlap integrals, M_C becomes

Appendix C

The following pages contain brief biographical sketches for Dr. M.A. Littlejohn and Dr. K.W. Kim.

BIOGRAPHICAL SUMMARY FOR MICHAEL A. LITTLEJOHN

Business Address

Department of Electrical and Computer Engineering
North Carolina State University
Box 7911
Raleigh, North Carolina 27695-7911
(919) 737-5247

Education

North Carolina State University	1962 B.S. Electrical Engineering
North Carolina State University	1964 M.S. Electrical Engineering
North Carolina State University	1967 Ph.D. Electrical Engineering

Industrial and Academic Experience

1967-present. Assistant Professor/Associate Professor/Professor,
Department of Electrical and Computer Engineering,
North Carolina State University, Raleigh, North
Carolina.

1977-1981, 1985-present. Technical Staff Member, U.S. Army
Research Office, Research Triangle Park,
North Carolina.

1981-1983. Director, Microelectronics Programs, School of
Engineering, North Carolina State University,
Raleigh, North Carolina.

1984-1985. Associate Dean of Engineering for Research
Programs, North Carolina State University, Raleigh,
North Carolina.

1988-1989. Associate Director, NSF Engineering Research Center
On Advanced Electronic Materials Processing.

Professional Activities

Member at Large, Executive Committee of the Electronics Division of
the Electrochemical Society, 1983-1988.

Member, National Academy of Sciences National Research Council
Committee on Recommendations for U.S. Army Basic Scientific
Research, 1985-1986.

Member, Technical Advisory Board, IEEE Engineering Research and Development Committee, 1986-1989.

Associate Editor, Electronics Division, Journal of the Electrochemical Society, 1987-1990.

Member, NSF Committee on Research Trends and Opportunities for the Metallurgy, Polymers, and Ceramics Section, Division of Materials Research, 1983-1985.

Organizer and Program Chairman, NSF Workshop on The Future of Microstructure Technology, 1985.

Co-organizer, NSF Workshop on Cooperation and Sharing Among U.S. Microelectronics Centers, 1983.

Society Memberships and Honors

Institute of Electrical and Electronics Engineers

American Society for Engineering Education

American Physical Society

Electrochemical Society

Certification of Achievement For Patriotic Civilian Service, U.S. Army, 1989.

R. J. Reynolds Industries, Inc., Award for Excellence in Teaching and Research, 1983-1987

Alcoa Foundation Distinguished Research Award, 1983

N. C. State University Alumni Award - University Distinguished Alumni Professor, 1980

Western Electric - ASEE Fund Award for Excellence in Teaching and Research (1978)

Sigma Xi Outstanding Young Scientist Award, 1976

Eta Kappa Nu Outstanding Teacher Award, 1974 & 1975

Field of Research Interest"

Semiconductor device simulation and modeling, III-V compound semiconductor materials and devices, hot electron transport in semiconductors, ion implantation and radiation damage in semiconductors, thin films and oxides on semiconductors, defects in semiconductors

Ten Most Recent Refereed Publications (From a total of 105)

1. D. L. Woolard, H. Tian, K. J. Trew, M. A. Littlejohn, and K. W. Kim, "A New Non-parabolic Hydrodynamic Model for Electron Transport in Semiconductors," accepted for publication in *Phys. Rev. B* (1991).
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Ki Wook Kim

Dept. of Electrical and Computer Engineering
Box 7911
North Carolina State University
Raleigh, NC 27695-7911

Phone: (919) 515-5229
FAX: (919) 515-3027

EDUCATION

- 08/88 Ph.D. in Electrical Engineering
 University of Illinois, Urbana, Illinois
 Thesis Title: Monte Carlo Studies of Nonlinear Electron Transport
 in III-V Semiconductors
- 05/85 M.S. in Electrical Engineering
 University of Illinois, Urbana, Illinois
- 02/83 B.S. in Electronics Engineering
 Seoul National University, Seoul, Korea

WORK EXPERIENCE

- 08/88 - present: Assistant Professor (Visiting), Department of Electrical and Computer Engineering, North Carolina State University, Raleigh, North Carolina
- 06/85 - 08/88: Graduate Research Assistant, Coordinated Science Laboratory, University of Illinois, Urbana, Illinois
- 06/83 - 05/85: Graduate Research Assistant, Department of Electrical Engineering, University of Illinois, Urbana, Illinois

ACADEMIC HONORS

IBM Predoctoral Fellowship (1986-1988)

RESEARCH INTERESTS

Semiconductor physics and modeling of electronic and optoelectronic devices, carrier transport in bulk and heterostructures, quantum effects, Monte Carlo simulation.

PUBLICATIONS

Refereed Articles in Journals

1. K. Kim, K. Kahen, J.P. Leburton, and K. Hess, "Band-Structure Dependence of Impact Ionization Rate in GaAs," *J. Appl. Phys.* 59, 2595 (1986).
2. K. Kim and K. Hess, "Simulations of Electron Impact Ionization Rate in GaAs in Nonuniform Electric Fields," *J. Appl. Phys.* 60, 2626 (1986).
3. D. Arnold, K. Kim, and K. Hess, "Effects of Field Fluctuation on Impact Ionization Rates in Semiconductor Devices due to the Discreteness and Distribution of Dopants," *J. Appl. Phys.* 61, 1456 (1987).
4. K. Kim, K. Hess, and F. Capasso, "New Effects of Structure in Momentum and Real Space on Nonlinear Transport across Heterojunction Band Discontinuities," *Appl. Phys. Lett.* 51, 508 (1987).
5. K. Kim, B. Mason, and K. Hess, "Inclusion of Collision Broadening in Semiconductor Electron Transport Simulations," *Phys. Rev. B* 36, 6547 (1987).
6. K. Kim, K. Hess, and F. Capasso, "Monte Carlo Study of Electron Heating and Enhanced Thermionic Emission by Hot Phonons in Heterolayers," *Appl. Phys. Lett.* 52, 1167 (1988).
7. M. Kuzuhara, K. Kim, D. Arnold, and K. Hess, "Ballistic Electron Transport across Collector Barriers in AlGaAs/GaAs Hot-Electron Transistors," *Appl. Phys. Lett.* 52, 1252 (1988).
8. K. Kim and K. Hess, "Ensemble Monte Carlo Simulations of Semiclassical Nonlinear Electron Transport across Heterojunction Band Discontinuities," *Solid-State Electron.* 31, 877 (1988).
9. K. Kim and K. Hess, "Electron Transport in AlGaAs/GaAs Tunneling Hot Electron Transfer Amplifiers," *J. Appl. Phys.* 64, 3057 (1988).
10. J. M. Higman, K. Kim, K. Hess, T. van Zutphen, and H. M. J. Boots, "Monte Carlo Simulation of Si and GaAs Avalanche Electron Emitting Diodes," *J. Appl. Phys.* 65, 1384 (1989).
11. M. Kuzuhara, K. Kim, and K. Hess, "Transient Simulation of AlGaAs/GaAs/AlGaAs and AlGaAs/InGaAs/AlGaAs Hot-Electron Transistors," *IEEE Trans. Electron Devices* ED-36, 118 (1989).
12. K. W. Kim, M. A. Strosio, and J. C. Hall, "Frequencies of Confined Longitudinal-Optical Phonon Modes in GaAs/GaP Short-Period Strained-Layer Superlattices," *J. Appl. Phys.* 67, 6179 (1990).
13. M. A. Strosio, K. W. Kim, and J. C. Hall, "Variation in Frequencies of Confined Longitudinal-Optical Phonon Modes due to Changes in the Effective Force Constants near Heterojunction Interfaces," *Superlatt. Microstruct.* 7, 115 (1990).
14. M. A. Strosio, K. W. Kim, M. A. Littlejohn, and H. Chuang, "Polarization Eigenvectors of Surface-Optical-Phonon Modes in a Rectangular Quantum Wire," *Phys. Rev. B* 42,

1488 (1990).

15. K. W. Kim and M. A. Strosio, "Electron-Optical-Phonon Interaction in Binary/Ternary Heterostructures," *J. Appl. Phys.* 68, 6289 (1990).
16. H. Tian, K. W. Kim, and M. A. Littlejohn, "Influence of DX Centers and Surface States on Delta-Doped High Electron Mobility Transistor Performance," *J. Appl. Phys.* 69, 4123 (1991).
17. K. W. Kim, H. Tian, and M. A. Littlejohn, "Analysis of Delta-Doped and Uniformly-Doped HEMTs by Ensemble Monte Carlo Simulation," *IEEE Trans. Electron Devices* ED-38, 1737 (1991).
18. M. A. Strosio, K. W. Kim, and S. Rudin, "Boundary Conditions for Electron-LO-Phonon Interaction in Polar Semiconductor Quantum Wires," *Superlatt. Microstruct.* 10, 55 (1991).
19. K. W. Kim, M. A. Strosio, A. Bhatt, R. Mickevicius, and V. V. Mitin, "Electron-Optical-Phonon Scattering Rates in a Rectangular Semiconductor Quantum Wire," *J. Appl. Phys.* 70, 319 (1991).
20. M. A. Strosio, G. J. Iafrate, K. W. Kim, M. A. Littlejohn, H. Goronkin, and G. Maracas, "Transition from Longitudinal-Optical Phonon Scattering to Surface-Optical Phonon Scattering in Polar Semiconductor Superlattices," *Appl. Phys. Lett.* 59, 1093 (1991).
21. D. L. Woolard, H. Tian, R. J. Trew, M. A. Littlejohn, and K. W. Kim, "A New Hydrodynamic Electron Transport Model: Nonparabolic Corrections to the Streaming Terms," accepted for publication in *Phys. Rev. B*.
22. H. Tian, K. W. Kim, and M. A. Littlejohn, "An Investigation of Doping Profile Variations on AlGaAs/GaAs High Electron Mobility Transistor Performance," accepted for publication in *J. Appl. Phys.*
23. R. Mickevicius, V. V. Mitin, K. W. Kim, M. A. Strosio, and G. J. Iafrate, "Electron Inter-subband Scattering by Confined and Localized Phonons in Real Quantum Wires," submitted to *Phys. Rev. B*.
24. H. Tian, K. W. Kim, M. A. Littlejohn, S. M. Bedair, and L. Witkowski, "Two-Dimensional Analysis of Short-Channel Delta-Doped GaAs MESFETs," submitted to *IEEE Trans. Electron Devices*.

Book Chapters

1. D. L. Woolard, H. Tian, M. A. Littlejohn, R. J. Trew, and K. W. Kim, "The Application of Monte Carlo Techniques in Advanced Hydrodynamic Transport Models," in *Monte Carlo Device Simulation: Full Band and Beyond*, edited by Karl Hess (Kluwer Academic Publishers, Boston, 1991), Chap. 8, pp. 219-266.

Refereed Articles in Proceedings of Conferences

1. K. Kim, K. Hess, and F. Capasso, "Simulations of Nonlinear Transport in AlGaAs/GaAs Single Well Heterostructures," presented at the 5th Int. Conf. on Hot Carriers in Semiconductors (July, 1987, Boston, Mass.), published in *Solid-State Electron.* 31, 349 (1988).
2. K. W. Kim, M. A. Strosio, and J. C. Hall, "Frequencies of Confined Longitudinal-Optical Phonon Modes in Short-Period Strained Semiconductor Superlattices," presented at the SPIE Int. Symp. on Optical & Optoelectronic Applied Science and Engineering (July, 1990, San Diego, Calif.), published in *SPIE Proceedings Series 1336*, 43 (1990).
3. M. A. Strosio, K. W. Kim, and M. A. Littlejohn, "Theory of Optical-Phonon Interactions in a Rectangular Quantum Wire (Invited)," presented at the SPIE Int. Conf. on Physical Concepts of Materials for Novel Optoelectronic Device Applications (October, 1990, Aachen, Germany), published in *SPIE Proceedings Series 1362*, 566 (1990).
4. M. A. Strosio, G. J. Iafrate, K. W. Kim, M. A. Littlejohn, H. L. Grubin, V. V. Mitin, and R. Mickevicius, "Role of Phonon Confinement in Nanoscale Systems (Invited)," presented at the Int. Symp. on Nanostructures and Mesoscopic Systems (May, 1991, Santa Fe, New Mexico), to be published in *Nanostructure Physics and Fabrication*.
5. R. Mickevicius, V. V. Mitin, K. W. Kim, and M. A. Strosio, "Electron Intersubband Scattering in Real Quantum Wires," presented at the Int. Symp. on Nanostructures and Mesoscopic Systems (May, 1991, Santa Fe, New Mexico), to be published in *Nanostructure Physics and Fabrication*.
6. K. W. Kim, M. A. Littlejohn, M. A. Strosio, and G. J. Iafrate, "Transition from LO-Phonon to SO-Phonon Scattering in Mesoscale Structures," presented at the 7th Int. Conf. on Hot Carriers in Semiconductors (July, 1991, Nara, Japan), to be published in *Semicond. Sci. Technol.*
7. R. Mickevicius, V. V. Mitin, K. W. Kim, and M. A. Strosio, "Electron High-Field Transport in Multi-Subband Quantum Wire Structures," presented at the 7th Int. Conf. on Hot Carriers in Semiconductors (July, 1991, Nara, Japan), to be published in *Semicond. Sci. Technol.*
8. S. Das Sarma, M. A. Strosio, and K. W. Kim, "Confined Phonon Modes and Hot Electron Energy Relaxation in Semiconductor Microstructures (Invited)," presented at the 7th Int. Conf. on Hot Carriers in Semiconductors (July, 1991, Nara, Japan), to be published in *Semicond. Sci. Technol.*
9. D. L. Woolard, H. Tian, M. A. Littlejohn, R. J. Trew, and K. W. Kim, "Impact of K-Space Transfer and Band Nonparabolicity on Electron Transport in a GaAs Ballistic Diode," presented at the 7th Int. Conf. on Hot Carriers in Semiconductors (July, 1991, Nara, Japan), to be published in *Semicond. Sci. Technol.*
10. U. K. Mishra, L. M. Jelloian, M. Lui, M. Thompson, S. E. Rosenbaum, and K. W. Kim, "Effect of n and p Channel Doping on the I-V Characteristics of AlInAs-GaInAs HEMTs," to be presented at the Int. Symp. on Gallium Arsenide and Related Compounds (September, 1991, Seattle, Washington), to be published in the Proceedings.

11. H. Tian, K. W. Kim, and M. A. Littlejohn, "Ensemble Monte Carlo Study of A Novel Heterojunction Real-Space Transfer Logic Transistor (RSTLT)," to be presented at the IEEE Int. Electron Devices Meeting (December, 1991, Washington, DC), to be published in *IEDM Tech. Digest*.
12. M. A. Stroscio, K. W. Kim, G. J. Iafrate, M. Dutta, and H. L. Grubin, "Reduction and Control of Inelastic Longitudinal-Optical Phonon Scattering in Nanoscale and Mesoscopic Device Structures (Invited)," to be presented at the 1991 Int. Semiconductor Device Research Symp. (December, 1991, Charlottesville, Virginia), to be published in the Proceedings.